

**OPTIMAL DESIGN AND SCHEDULING OF UNSTEADY STATE MATERIAL  
RECOVERY NETWORKS**

A Dissertation

by

ARWA H. RABIE

Submitted to the Office of Graduate Studies of  
Texas A&M University  
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

December 2008

Major Subject: Chemical Engineering

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**ABSTRACT**

Optimal Design and Scheduling of Unsteady State Material Recovery Networks.

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Chair of Advisory Committee: Dr. Mahmoud M. El-Halwagi

This research developed novel methodologies to achieve cost effective solutions to overcome many of the difficulties associated with unsteady state material recovery network synthesis. The work focuses on the development of three different methodologies: the first is a hierarchical multi-step methodology developed for the design and scheduling of batch water (material of interest) recycle networks. A new source- double tank-sink arrangement is introduced to overcome the limitation of same-cycle assignment by permitting sources to be optimally recycled within the same batch cycle and/or storing and recycling sources to sinks in the following batch cycle. The problem is solved in interconnected stages. First, network targets such as minimum fresh water consumption and minimum waste water discharge are identified ahead of network design. Once design targets have been identified, an iterative procedure is followed to tradeoff fixed and operating cost to achieve a network design which has the minimum total annualized cost (TAC).

The second developed methodology is a one-step simultaneous approach to design and schedule cost-effective batch water recycle networks. A new source-tank-sink representation is developed to embed potential configurations of interest for design and scheduling. As a result, water may be assigned from sources to sinks within the same cycle (with or without a storage tank) and in two subsequent cycles using a double tank arrangement. A mathematical formulation is developed to determine the network design and sufficient information on the scheduling of the network with the minimum TAC in one step.

The third methodology this research developed is a systematic procedure to schedule the operation of an unsteady state material recovery network. The network has a set design and receives a number of feedstocks (sources) that are to be processed into higher value/quality products. The sources may be stored in tanks, mixed, and/or intercepted in separation devices to produce the desired products while maximizing profits and meeting all process constraints. The developed systematic procedure includes mathematical formulations that allow available sources to be stored, mixed, intercepted and determine the optimal scheduling scheme over time period  $\tau$  with the objective of maximizing total annualized profit of the network.

*Dedicated to*  
*My parents Hamed and Laila Rabie*  
*and my Brothers Basil and Feras*  
*with Love*

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## **CHAPTER I**

### **INTRODUCTION**

In conventional chemical process design methodologies, different units or network of units are designed individually, and then the units or network of units are linked together. Depending on the way the units are connected, the overall optimal process design may or may not be achieved. This unit-based approach can lead to operational difficulties when, as an example, the need to alter the process operating conditions arises. Moreover, local equipment failure can significantly impact the performance of the entire plant, and maintenance activities can be complicated (Linnhof et al., 1982). Furthermore, this approach can lead to a higher cost associated with a poor overall process performance, inefficient use of valuable resources, excessive waste generation, and a negative environmental impact.

In recent years, a holistic approach to process design and operation has been developed. This approach, known as process integration, focuses on the unity of the overall process design and operation of all units involved within the process rather than focusing on individual units and then linking different units or network of units together (Dunn

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This dissertation follows the style and format of Chemical Engineering Science.

and El-Halwagi, 2003). Moreover, it identifies optimal performance targets for the overall process before the detailed design of the network is developed. The design scheme that satisfies the pre-identified targets is considered to be the optimum design solution. Pre-identifying performance targets leads to a more efficient design methodology that requires less time to develop. This is particularly important, as conventional process design methodologies are time consuming and use detailed computational and iterative approaches.

This approach enabled researchers to develop systematic procedures and methodologies for sustainable development, optimal design, operational efficiency, debottlenecking, resources conservation, yield enhancement, as well as waste reduction which results in significant cost reduction for industrial facilities, and an observable benign impact on the environment. To achieve that, a set of graphical and computer-aided optimization tools are developed and utilized.

The newly developed research area was inspired by the work of Linnhof in 1982. He introduced this concept to the design of heat exchangers in order to optimize the use of fuel and energy and reduce the capital and operating cost associated with that. This heat integration methodology was further expanded by the development of the thermal pinch analysis. Depending on the type of the utility, the optimum heating loads to be added or cooling loads to be removed will be determined taking in considerations the optimum streams pairing, mixing, and/or splitting (Dunn and El-Halwagi, 2003).

An important area of process integration, known as property integration, was recently introduced by El-Halwagi's research group (Shelley & El-Halwagi, 2000; El-Halwagi et al., 2004). El-Halwagi et al. defined this "component-independent design" concept as "a functionality-based, holistic approach to the allocation and manipulation of streams and processing units which is based on tracking, adjustment, assignment, and matching of functionalities throughout the process" (Dunn and El-Halwagi, 2003).

In a significant development in 1989, the process integration concept was extended by El-Halwagi and Manousiouthakis to a new dimension by the development of the mass integration approach. "Mass integration can be defined as a holistic approach to the generation, separation, and routing of species and streams throughout the process. It is a systematic methodology that provides a fundamental understanding of the global flow of mass within the process, and employs it in identifying performance targets and optimizing the allocation and generation of streams and species with the objectives of enhancing yield, conserving resources, debottlenecking, mitigating environmental impact, and conserving energy." (El-Halwagi and Manousiouthakis, 1989; Dunn and El-Halwagi, 2003)

The introduction of this powerful methodology and new concept in process design enabled researchers in the field to investigate numerous industrial issues and develop effective solutions for complex problems. Polley and Polley, 2000, investigated industrial operations that demand quantity-controlled water systems and the trade-offs

between minimum water consumption and network complexity, operability, and capital cost. Bagajewicz and Savelski, 2001, used linear programming to develop a method for the optimum design of water networks with single contaminant. Sorin and Bedard, 1999, presented the Global Pinch Concept, which separates the design problem into two independent parts and enables to generate different water reuse network designs.

Many other techniques for water recycle and reuse networks have been reported by different research groups such as water pinch analysis by Wang and Smith, 1994; Hallale, 2002; Savelski and Bagajewicz, 2000a, source-sink graphical methodology by El-Halwagi, 1997; Dunn and Dobson, 1999, and Mathematical programming approaches by Alva-Argaez', et al., 1999; Keckler and Allen, 1998; Parthasarathy et al., 2001.

The high demand on resources and fresh streams in chemical plants and manufacturing facilities makes it inevitable to seek effective engineering solutions to conserve resources and increase material recovery. In addition, the increasingly stringent environmental regulations and constraints on waste streams discharge, requires the chemical industry to develop technically-capable and cost effective design schemes that meet the environmental standards and maintain profitability.

It is important to identify the sources of contaminant generation in the system before exerting effort to develop waste recovery processes and systems. If the source of contaminants is coming from within the process itself, such that the reaction pathways

lead to producing undesirable components that are considered to be contaminants, then the effort should be focused on developing alternative reaction pathways that produce contaminant free streams. If the source of the contaminant is not the process, then a more environmentally friendly component should be used. If it is infeasible to replace the contaminant in the process, then waste minimization, waste interception and allocation networks and methodologies should be developed (Wang and Smith, 1994; Dunn and Dobson, 1999; Huang and Edgar, 1995; Dunn and El-Halwagi, 2003).

Mass integration methodologies are effective tools utilized to achieve this goal. A mass-integration-based network synthesis provides cost effective and engineering capable solutions by answering a set of critical questions related to defining waste material streams and their optimal loads that need to be recycled, optimal allocation of the waste streams that need to be routed to the process, and what kind of arrangement need to be configured (Dunn and El-Halwagi, 2003).

Mass-exchange networks (MEN) synthesis, for example, is among the tools to be considered to identify cost-effective waste separation systems. A mass-exchange unit, which can be an extraction unit, an ion-exchange unit, an absorption column...etc., utilizes counter-current direct-contact design that exploits a mass-separating agent (MSA) to effectively decontaminate waste streams. The collective performance of mass exchange units which form the MEN is set to meet the requirements for waste stream decontamination level. The choice of the MSA along with identifying the optimal mass



load to be removed by the MSA and how the MSA stream will be matched with the waste stream are key factors for the synthesis of an effective MEN. (Dunn and El-Halwagi, 2003).

This research utilizes mass integration design tools to address challenging problems in the field, overcome serious limitations in previous research efforts, and develop a generally-applicable optimization-based methodology and a systematic procedure for the design, synthesis, and scheduling of cost-effective unsteady state material recovery networks while meeting all process constraints.

To date, the majority of material recovery network research has focused on continuous, steady-state processes (e.g., El-Halwagi, 2006; El-Halwagi et al., 2003; Mann and Liu, 2000; Bagajewicz, 2000). Unlike steady state network synthesis, dealing with unsteady state synthesis is more complicated and presents more challenges and obstacles to overcome. The dynamic behavior of unsteady state networks makes it a difficult task to synthesize a cost effective and optimal material recovery network.

In this research novel methodologies were developed to achieve cost effective solutions and to overcome many of the difficulties associated with unsteady state network synthesis. Moreover, significant effort was dedicated to developing cost effective solutions and formulations to the synthesis of batch networks to minimize fresh stream

consumption, and waste discharge. This is particularly important as batch systems are common in the industry and less attention has been given to them over the years.

Chapter II of this dissertation presents an overview of the overall problem statement. Chapter III illustrates the design and scheduling of cost effective batch water-recycle networks through a hierarchical approach. Chapter IV presents a simultaneous one step approach for designing and scheduling a cost effective unsteady state material recovery network. Chapter V demonstrates a process integration approach to the optimal scheduling of unsteady state material recovery networks. Chapter VI presents the summary and conclusion of this research.

## CHAPTER II

### PROBLEM STATEMENT

The overall problem considered in this research addresses the optimization of the synthesis, scheduling, and operation of unsteady state material recovery networks. The problem is stated as follows:

During an unsteady state material recovery process with a given cycle time ( $\tau$ ), there are a number of sources and sinks characterized by the following:

- Sources: There is a set  $SOURCES = \{v | v = 1, 2, \dots, N_{SR}\}$  of process streams that contain the material of interest. The dynamic profiles for the flow rate and composition of each source,  $v$ , are known and given by  $w_v(t)$  and  $y_{v,u}(t)$  where  $u$  is an index for components and  $t$  is the time from the beginning of the cycle ( $0 \leq t \leq \tau$ ).
- Sinks: There is a set  $SINKS = \{s | s = 1, 2, \dots, N_{SK}\}$  of process units that require the material of interest. Constraints on dynamic profiles for the flow rate and maximum admissible composition of impurity  $u$ , of each sink  $s$ , are known and given by  $g_s(t)$  and  $z_{s,u}^{max}(t)$ .

Available for service are:

- A number of fresh streams; each fresh stream  $h$  has a given concentration of the  $u^{th}$  impurity designated by  $x_{h,u}$ .

It is desired to develop a systematic procedure to synthesize and schedule an unsteady state material recovery network in which the material of interest from sources may be stored in tanks then recycled to sinks when needed or released as waste. The network must be cost effective and meet all process constraints. The synthesis and scheduling tasks require the identification of the following:

- What is the optimum network configuration including assignment of sources and sinks?
  - Which fresh stream(s) should be used? How much of each?
  - How many tanks should be used? What are their sizes? What are their feeds?
- How should the synthesized network be scheduled for operation?

Designers are often faced with the need to optimally synthesize and schedule material recovery networks. However, in other realistic scenarios the need arises to develop an optimal scheduling for operating existing material recovery networks with a set number of tanks, pipelines, and a set overall network design. The following is a problem statement that deals with such scenarios:

Given is a process with a number of interception units, tanks, and pipelines. The process receives various batches of feedstocks that are to be processed to produce a number of value-added/higher quality products that meet certain market demands. It is desired to determine optimal scheduling strategies for the allocation and separation of the

feedstocks over a decision making time horizon  $\tau$ . The above is characterized by the following:

- Sources: There is a set of sources  $SOURCES = \{i|i = 1, 2, \dots, N_{SR}\}$  of process streams containing the material of interest that needs to be recovered. The dynamic profiles for the flow rate and composition of each source,  $i$ , are known only over  $\tau$  and given by  $a_i(t)$  and  $v_i(t)$  where  $t$  is the time during period  $\tau$ .
- Interceptors: There is a set of existing interceptor units  $INTERCEPTORS = \{n|n = 1, 2, \dots, N_{INT}\}$  with a set type, size, and design. These units can intercept the sources in order to recover the material of interest. There are also capacity and composition limitations on the feed to each interceptor and are given by

$$F_n^{in, \min} \leq F_n^{in} \leq F_n^{in, \max} \text{ and } X_n^{in, \min} \leq X_n^{in} \leq X_n^{in, \max} \text{ respectively.}$$

- Tanks: There are two sets of tanks  $TANKS_1 = \{k|k = 1, 2, \dots, N_{TK1}\}$  and  $TANKS_2 = \{m|m = 1, 2, \dots, N_{TK2}\}$  with a set location and capacity.  $TANKS_1$  can be used to store the sources before interception and have a capacity  $T_k^1$ .  $TANKS_2$  store sources after interception and have a capacity  $T_m^2$ .
- Products: There is a set of products  $PRODUCTS = \{j|j = 1, 2, \dots, N_{PD}\}$  with certain specifications that need to be produced from the recovered material. The flow rate and composition constraints on the desired product are given by:

$$P_j^{\min}(t) \leq P_j(t) \leq P_j^{\max}(t) \text{ and } Z_j^{\min}(t) \leq Z_j(t) \leq Z_j^{\max}(t)$$

The objective is to develop a systematic procedure to determine the optimal scheduling schemes for the optimal material recovery network over time period  $\tau$  in which sources may be stored in tanks, mixed, and/or intercepted to produce the desired products. The material recovery network must produce the maximum profits and meet all process constraints.

## **CHAPTER III**

### **SYNTHESIS AND SCHEDULING OF OPTIMAL BATCH WATER-RECYCLE NETWORKS**

#### **3.1 Introduction**

Water conservation is an important industrial objective. It contributes to the conservation of natural resources, reduction of negative environmental impact, and optimization of the cost of water usage and discharge. While much work has been undertaken in the area of designing water networks for steady-state applications (recent reviews includes El-Halwagi, 2006; El-Halwagi et al., 2003; Mann and Liu, 2000; Bagajewicz, 2000), much less work has been done on batch water processes. Given that batch systems are common within industry, it is important to develop batch water recycle networks that minimize fresh water consumption and wastewater discharge.

Wang and Smith, 1995, developed a time-pinch analysis method which uses graphical techniques to synthesize batch water networks. Majozi et al., 2006, also devised a graphical technique which is an extension of the time-pinch analysis technique. In these works, water-using units are modeled as mass exchangers to deal with single-contaminant systems. Foo et al., 2005, developed the water cascade analysis. In this method, mixing of water sources at different impurities in the same tank is not allowed.

Kim and Smith, 2004, and Majozi, 2005a, b, developed mathematical formulations that optimize water usage and network configuration. These formulations are limited to mass transfer based water units and single contaminant systems. Chang and Li, 2006, also developed a mathematical formulation for batch networks that are not limited to mass transfer based water units. Despite the significance of the contributions achieved by previous research, the following serious hurdles and limitations are still to be overcome:

- Recycle within the same cycle
- Lumped usage of water over a cycle
- Limited objective (e.g., fresh-water minimization)

The research presented in this dissertation addresses these limitations and provides effective solutions. This work develops a systematic procedure to synthesize and schedule a cost effective batch water network. A source-tank-sink structural representation is developed to account for the potential configurations of the water network. A hierarchical procedure is developed to solve the problem in interconnected stages and to establish trade offs between capital and operating costs.

This work also introduces novel ways to overcome all the aforementioned limitations. First, the limitation of same-cycle assignment is removed by permitting sources to be optimally recycled within the same batch cycle and/or storing and recycling sources to sinks in the following batch cycle. Second, the limitation of lumped usage of water over a cycle is avoided by implementing a two-tank arrangement when needed to allow for



proper scheduling of recycled source water to sinks. Third, the objective function is extended to include the minimization of both the operating cost (fresh water) as well as the fixed cost of the network.

### 3.2 Nomenclature

$C_r$	Cost of fresh water stream $r$
$f_{r,j}$	Flow of fresh water from stream $r$ to discretized sink $j$
$G_j$	Water demand of discretized sink $j$
$I_k$	Zero/one binary integer variable designating absence/existence of tank $k$
$N_q$	Number of multiple time periods per cycle
$N_{sources}$	Number of discretized sources
$N_{sinks}$	Number of discretized sinks
$N_{SK}$	Number of process sinks
$N_{SR}$	Number of process sources
$t$	Time
$T_k$	Water capacity of tank $k$
$t_{k,j}$	Water flow from tank $k$ to discretized sink $j$
$U_k$	Upper bound on maximum capacity of tank $k$
$W$	Total waste water

$W_i$	Water flow of discretized source $i$
$w_{i,j}$	Water flow from discretized source $i$ to discretized sink $j$
$w_{i,k}$	Water flow from discretized source $i$ to tank $k$
$w_{i,waste}$	Water flow from discretized source $i$ to waste
$x_{r,u}$	Composition of component $u$ in fresh water stream $r$
$Y_{i,u}$	Composition of component $u$ in discretized source $i$
$y_{k,u}^{Tank}$	Composition of component $u$ in tank $k$
$z_{j,u}$	Composition of component $u$ in discretized sink $j$
$z_{j,u}^{max}$	Maximum admissible composition of component $u$ to discretized sink $j$

### 3.2.1 Subscripts

$I$	Discretized sources
$j$	Discretized sinks
$k$	Storage and dispatch tanks
$q$	Discretization index for time intervals
$r$	Fresh water stream
$s$	Sinks
$u$	Component
$v$	Sources

### 3.3 Problem Statement

The batch water network problem to be addressed in this work may be stated as follows:

During a batch process with a given cycle time ( $\tau$ ), there are a number of water sources and sinks characterized by the following:

- Sources: There is a set  $\text{SOURCES} = \{v | v = 1, 2, \dots, N_{\text{SR}}\}$  of process water streams. The dynamic profiles for the flow rate and composition of each source,  $v$ , are known and given by  $w_v(t)$  and  $y_{v,u}(t)$  where  $u$  is an index for components and  $t$  is the time from the beginning of the cycle ( $0 \leq t \leq \tau$ ).
- Sinks: There is a set  $\text{SINKS} = \{s | s = 1, 2, \dots, N_{\text{SK}}\}$  of process units that require water. Sinks can be a variety of units including washers, separators, reactors, etc. Constraints on dynamic profiles for the flow rate and maximum admissible composition of impurity of each sink  $s$  are known and given by  $g_s(t)$  and  $z_{s,u}^{\max}(t)$ .

Available for service are:

- A number of fresh water streams; each fresh stream  $r$  has given concentration of the  $u^{\text{th}}$  impurity designated by  $x_{r,u}$ .

It is desired to develop a systematic procedure to synthesize and schedule a batch water network in which water from sources may be stored in tanks then recycled to sinks when needed or released as waste. The water network must be cost effective and meet all process constraints.

### 3.4 Approach

The following hierarchical procedure is proposed:

1. Targeting minimum usage of fresh water and minimum wastewater discharge
2. Synthesis of a direct-recycle water network using storage and dispatch tanks to achieve the target
3. Scheduling of an optimum operating scheme to achieve the target
4. Tradeoff between fixed and operating costs

The details of the proposed procedures are described in the following sections.

#### 3.4.1 Multiperiod Reformulation of Sources and Sinks

To avoid dealing with dynamic differential equations for sources and sinks, transformation to algebraic equations is undertaken via discretization. The discretization index is referred to as  $q$ . The  $q^{\text{th}}$  time interval between indices  $q-1$  and  $q$  is described by the following time interval  $[t_{q-1}$  and  $t_q]$ . For the  $q^{\text{th}}$  time interval, the quantity of the  $v^{\text{th}}$  source is given by:

$$W_{v,q} = \int_{t_{q-1}}^{t_q} w_v(t) dt \quad (3.1)$$

and the composition of the  $u^{\text{th}}$  component is given by

$$y_{v,q,u} = \frac{\int_{t_{q-1}}^{t_q} w_v(t) y_{v,u}(t) dt}{W_{v,q}} \quad (3.2)$$

To simplify the terminology, a single index,  $i$ , will be used for all discretized sources such that  $i = 1$  corresponds to  $v = 1$  and  $q = 1$ ,  $i = 2$  corresponds to  $v = 1$ ,  $q = 2$ , and so on until  $i = N_{\text{Sources}}$  corresponds to  $v = N_{\text{SR}}$  and  $q = N_{\text{t\_Sources}}$ . For each discretized source  $i$ , the flow and composition are referred to by  $W_i$  and  $Y_{i,u}$ . Similarly, for the constraints on the sinks:

$$G_{s,q} = \int_{t_{q-1}}^{t_q} g_s(t) dt \quad (3.3)$$

and the composition constraints are given by:

$$z_{s,q,u}^{\max} = \frac{\int_{t_{q-1}}^{t_q} g_s(t) z_{s,u}^{\max}(t) dt}{G_{s,q}} \quad (3.4)$$

Again, to simplify the index terminology, a single index,  $j$ , will be used for all discretized sink constraints such that  $j = 1$  corresponds to  $s = 1$  and  $q = 1$  until  $j = N_{\text{Sinks}}$  which corresponds to  $s = N_{\text{SK}}$  and  $q = N_{\text{t\_Sinks}}$ . For each discretized sink  $j$ , the flow and composition constraints are referred to by  $G_j$  and  $Z_{j,u}^{\max}$ .

The structural representation involves the discretized sources and sinks as well as up to two sets of tanks: one for storage and one for dispatch. When the two sets are used, they alternate roles with storage in one cycle and dispatch in the subsequent cycle. For the special case where only storage and dispatch tanks dominate the fixed cost of the network and fresh water and waste water treatment dominate the operating cost of the network, a hierarchical procedure is developed for this special case to solve the problem in interconnected stages. Benchmarks for minimum usage of fresh water and wastewater discharge are determined by eliminating scheduling constraints. An iterative procedure is formulated to minimize the total annualized cost of the system by trading off capital versus operating costs.

### 3.4.2 Targeting for Minimum Fresh Usage and Wastewater Discharge

The first step in the developed hierarchical procedure for the special case, where tanks dominate the fixed cost of the network, is to determine benchmarks for the operating cost of the network by identifying lower bounds for the usage of fresh water and the discharge of wastewater. One target is to determine the minimum flow of the fresh (which also corresponds to minimum discharge of the wastewater):

$$\text{Minimize } \sum_{r=1}^{N_{Fresh}} \sum_{j=1}^{N_{sinks}} f_{r,j} \quad (3.5a)$$

where  $f_{r,j}$  is the flow rate of the  $r^{\text{th}}$  fresh assigned to the  $j^{\text{th}}$  sink. Another objective is to determine the minimum cost of the fresh as follows:

$$\text{Minimize } \sum_{r=1}^{N_{\text{Fresh}}} \sum_{j=1}^{N_{\text{Sinks}}} C_r f_{r,j} \quad (3.5b)$$

Subject to Splitting of sources:

$$W_i = \sum_{j=1}^{N_{\text{Sinks}}} w_{i,j} + w_{i,\text{waste}}, \quad i=1, 2, \dots, N_{\text{Sources}} \quad (3.6)$$

Waste flow:

$$W = \sum_{i=1}^{N_{\text{Sources}}} w_{i,\text{waste}} \quad (3.7)$$

Sink balances:

$$G_j = \sum_{i=1}^{N_{\text{Sources}}} w_{i,j} + \sum_{r=1}^{N_{\text{Fresh}}} f_{r,j}, \quad j=1, 2, \dots, N_{\text{Sinks}} \quad (3.8)$$

$$G_j Z_{j,u} = \sum_{i=1}^{N_{\text{Sources}}} w_{i,j} Y_{i,u} + \sum_{r=1}^{N_{\text{Fresh}}} f_{r,j} x_{r,u}, \quad j=1, 2, \dots, N_{\text{Sinks}} \text{ and } u=1, 2, \dots, N_{\text{Components}} \quad (3.9)$$

Composition constraints for the Sinks:

$$Z_{j,u} \leq Z_{j,u}^{\max}, \quad j=1,2,\dots,N_{\text{Sinks}} \text{ and } u=1,2,\dots,N_{\text{Components}} \quad (3.10)$$

### 3.4.3 Minimizing Fixed Cost

The next step is to synthesize and schedule a batch water network in which the fixed cost is minimized while still meeting the water targets determined in the previous step. The items which dominate the fixed cost are the storage and dispatch tanks. Therefore, the quantity of tanks is minimized using the following objective function:

$$\text{Minimize } \sum_{k=1}^{N_{\text{Tanks}}} 2I_k \quad (3.11)$$

where  $I_k$  is a zero/one binary integer variable designating the absence/existence of a tank.

The following constraints are used:

Splitting of Sources:

$$W_i = \sum_{k=1}^{N_{\text{Tanks}}} w_{i,k} + w_{i,\text{waste}}, \quad i=1,2,\dots,N_{\text{Sources}} \quad (3.12)$$



Storage-tank balances:

$$T_k = \sum_{i=1}^{N_{Sources}} w_{i,k} , \quad k=1,2,\dots,N_{Tanks} \quad (3.13)$$

$$T_k y_{k,u}^{Tank} = \sum_{i=1}^{N_{Sources}} w_{i,k} Y_{i,u} \quad k=1,2,\dots,N_{Tanks} \text{ and } u=1,2,\dots,N_{Components} \quad (3.14)$$

$$T_k = \sum_{j=1}^{N_{sinks}} t_{k,j} , \quad k=1,2,\dots,N_{Tanks} \quad (3.15)$$

Waste flow:

$$W = \sum_{i=1}^{N_{sources}} w_{i,waste} \quad (3.16)$$

Sink balances:

$$G_j = \sum_{k=1}^{N_{Tanks}} t_{k,j} + \sum_{r=1}^{N_{Fresh}} f_{r,j} , \quad j=1,2,\dots,N_{Sinks} \quad (3.17)$$

$$G_j Z_{j,u} = \sum_{k=1}^{N_{Tanks}} t_{k,j} y_{k,u}^{Tank} + \sum_{r=1}^{N_{Fresh}} f_{r,j} x_{r,u} , \quad j=1,2,\dots,N_{Sinks} \text{ and } u=1,2,\dots,N_{Components} \quad (3.18)$$

Composition constraints for the Sinks:

$$Z_{j,u} \leq Z_{j,u}^{\max}, \quad j=1,2,\dots,N_{\text{Sinks}} \text{ and } u=1,2,\dots,N_{\text{Components}} \quad (3.19)$$

Fresh flow:

$$Fresh = \sum_{r=1}^{N_{Fresh}} \sum_{j=1}^{N_{sinks}} f_{r,j} \quad (3.20)$$

Furthermore, two more constraints are needed. First, assigning the integer values to used tanks: since the variable  $I_k \in \{0,1\}$ , it is necessary to add a constraint which assigns the value zero when there is no feed to the tank and one when there is feed to the tank. This can be accomplished by the following constraint:

$$T_k \leq U_k I_k, \quad k=1,2,\dots,N_{\text{Tanks}} \quad (3.21)$$

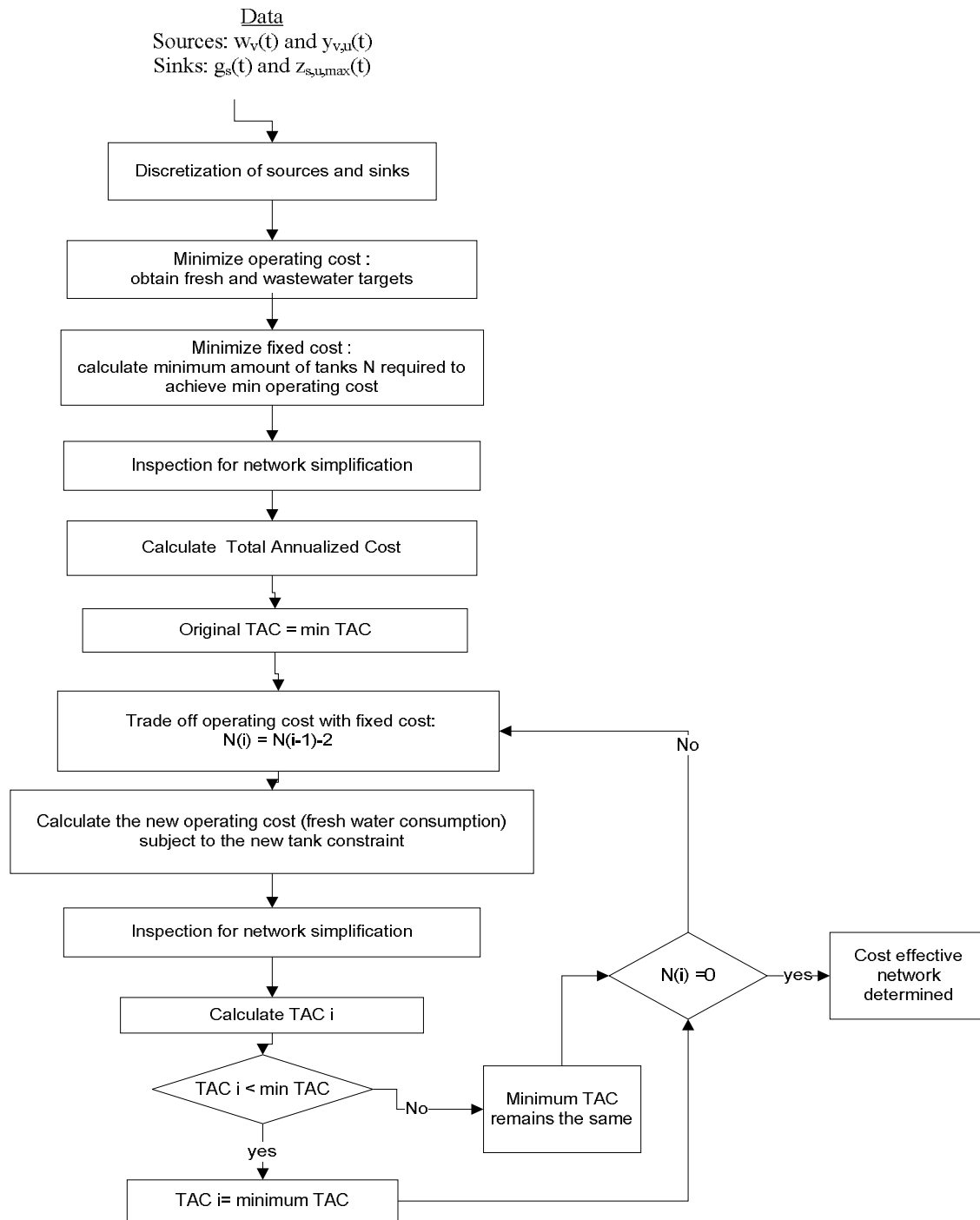
where  $U_k$  is a given upper bound on the maximum capacity of the tank. When there is positive flow ( $T_k$ ) to tank  $k$ , the variable  $I_k$  is forced to be one. On the other hand, when  $T_k$  is zero, the constraint is satisfied by  $I_k$  being zero or one. However, the zero value will be picked in order to minimize the objective function.

Second, a constraint is added to include the value of the operating cost (either the minimum fresh cost target identified earlier or an iterative target for trading off fixed versus operating costs as will be described in the next section). Hence,

$$\sum_{r=1}^{N_{Fresh}} \sum_{j=1}^{N_{sinks}} C_r f_{r,j} = \text{Cost} \quad (3.22)$$

#### 3.4.4 Minimizing Total Annualized Cost (TAC)

The last step in attaining a cost effective batch water network for the special case where tanks dominate the fixed cost of the network, is to achieve the minimal TAC of the system by trading off fixed and operating costs. The proposed approach is shown by Fig. 3.1. First, the problem of minimizing the operating cost (minimizing fresh water consumption) is solved. The solution of this program provides the targets for fresh flow and wastewater discharge. Next, the fixed-cost minimization problem is solved subject to the identified fresh target. The solution identifies the assignment of sources to tanks and tanks to sinks, the associated flows, and the scheduling scheme. Inspection of the new design is done to try to further simplify the network. The solution is inspected to see if the two sets of tanks are needed for each assignment. If scheduling of any assignment can be done in one tank or without tanks, the unnecessary tanks are eliminated. Now that the network configuration has been determined, the TAC corresponding to this system can be calculated. Next, tradeoff of operating cost with fixed cost is done by decreasing



the quantity of tanks used in the network by two. Then, the minimum operating cost (fresh water consumption) subject to the new tank constraint is determined. Further inspection of the new design is done to try to simplify the network. Comparison of the original TAC and the new TAC is carried out. If the new annualized cost is lower than the original, it will replace the original total annualized cost as the current minimum. If not, the original TAC remains as the current minimum. Iterations are continued until a system of zero tanks is achieved (corresponding to the minimum fixed cost and maximum operating cost). The minimum stored value of the TAC is the most cost effective network and it provides sufficient information on the associated configuration and scheduling schemes.

### **3.5 Case Study**

Consider a batch process with water sources and sinks. Tables 3.1 and 3.2 summarize the data for the sources and sinks. Available for use is one fresh water stream with a cost of \$0.20/ton of water. Also, the cost of waste water treatment is \$0.30/ton. Available are storage and dispatch tanks with an annual cost of \$35,000 per tank and associated piping.

First, the dynamic profiles of sources and sinks are transformed into multi-period data by discretizing and integrating over eight equal intervals (1 hr each). To determine the network with the minimum target for fresh water usage and wastewater discharge, one must determine the minimum operating cost using the first mathematical formulation.

Table 3.1

Data for the Process Sources of the Case Study ( $t$ : time (hr) from the start of the cycle)

Source Number	Function for Flow Rate (ton/hr)	Function for Composition (ppm)	Start Time (hr)	End Time (hr)
1	200.00	$40 * t + 40$	0	5
2	133.33	$10 * (t - 1)^2 + 20$	1	4
3	$(15.00 * (t - 7) + 70.00) * 10$	300	7	8

Table 3.2

Data for the Process Sinks of the Case Study

Sink Number	Flow rate Demand (ton/hr)	Constraint on Lower Bound on Composition Entering the Sink (ppm)	Constraint on Upper Bound on Composition Entering the Sink (ppm)	Start Time, (hr)	End Time, (hr)
1	290.00	0	80	1	6
2	100.00	0	350	3	7

The formulation is a linear program whose global solution provides 250 ton of fresh water and 575 ton of wastewater per batch cycle with a yearly operating cost of \$243,637. Next, the hierarchical procedure was employed to trade off capital versus operating costs and to schedule and configure the network. Three iterations were performed with networks featuring four tanks, two tanks, and no tanks and the resulting total annualized costs for these three configurations were found respectively to be \$383,637, 377,388, and 545,698. Therefore, the solution of \$377,388/yr was selected. This network consists of 2 tanks, consumes 366.5 tons of fresh water and generates 691.4 tons of waste water per batch cycle.

To further demonstrate the results of the optimized network, Figs. 3.2 and 3.3 along with Table 3.3, are illustrations of the original unintegrated network and the optimized network respectively. Comparing the annual cost of both networks, it is evident that it is economically beneficial to implement a batch water recycle network.

To further investigate optimization, sensitivity analysis is done on the price of fresh water. Fig. 3.4 illustrates the sensitivity of fresh water price. As the cost of fresh water increases, both the operating cost as well as the TAC of the network increase. This increase has an effect on the optimization of the batch water recycle network. When the cost of fresh water is \$0.1/ton or \$0.2/ton, it is determined that the optimal network is a network made up of two tanks and consumes 366.5 tons of fresh water per batch cycle.

When the cost of fresh water increases to, for example, \$0.5/ton or \$0.7/ton, the optimal network is no longer a network of two tanks. Instead, the optimal design is a network of four tanks which consumes the minimum fresh water target of 250 tons of fresh water per batch cycle.

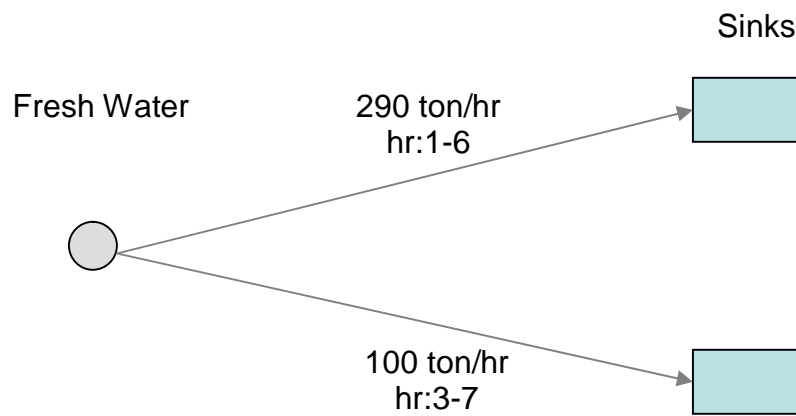


Fig. 3.2. Original Unintegrated Network with a TAC of \$1,119,634



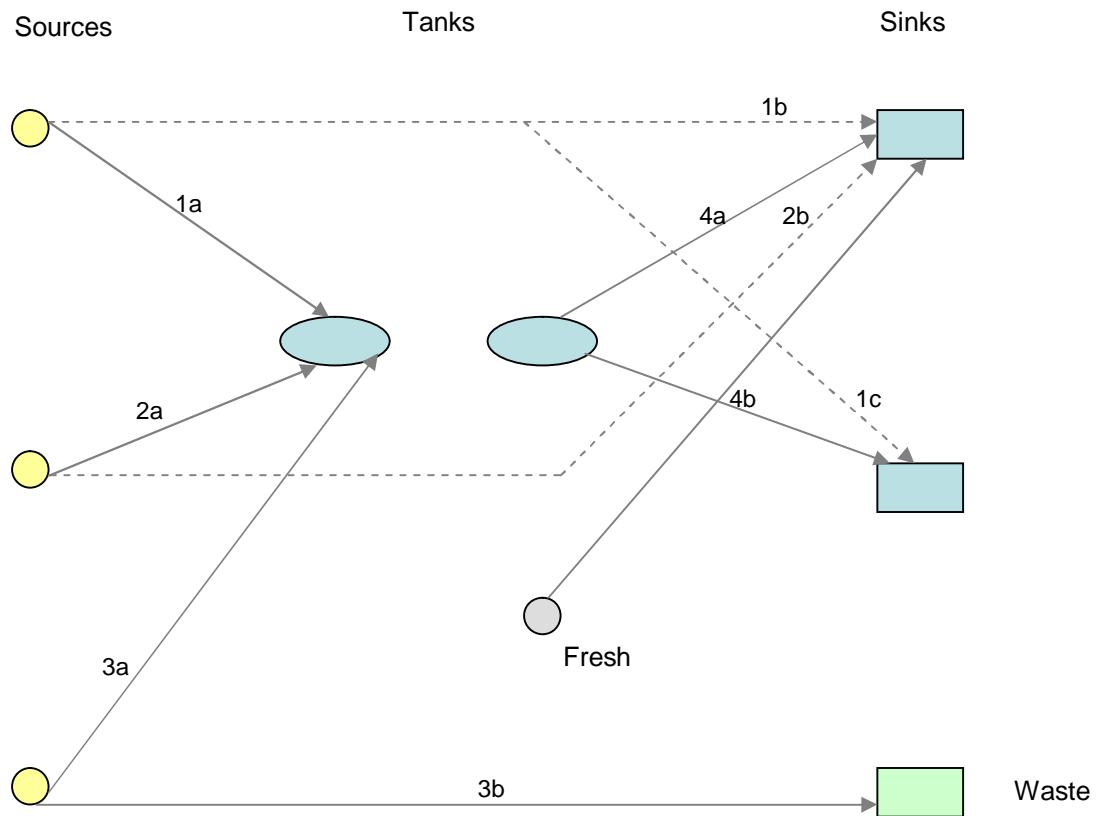


Fig. 3.3. Optimized Batch Water Recycle Network with a TAC of \$377,388

Table 3.3

Legend for Fig. 3.3

Time Interval (hr)	1a (ton)	1b (ton)	1c (ton)	2a (ton)	2b (ton)	3a (ton)	3b (ton)	4a (ton)	4b (ton)	5a (ton)
0-1	200	-----	-----	-----	-----	-----	-----	-----	-----	-----
1-2	-----	200	-----	52.32	80.99	-----	-----	9.01	-----	-----
2-3	75.5	124.5	-----	-----	133.33	-----	-----	-----	-----	32.34
3-4	100	-----	100	-----	133.33	-----	-----	83.2	-----	73.5
4-5	100	-----	100	-----	-----	-----	-----	160	-----	130.4
5-6	-----	-----	-----	-----	-----	-----	-----	160	100	130.4
6-7	-----	-----	-----	-----	-----	-----	-----	-----	100	-----
7-8	-----	-----	-----	-----	-----	83.58	691.4	-----	-----	-----

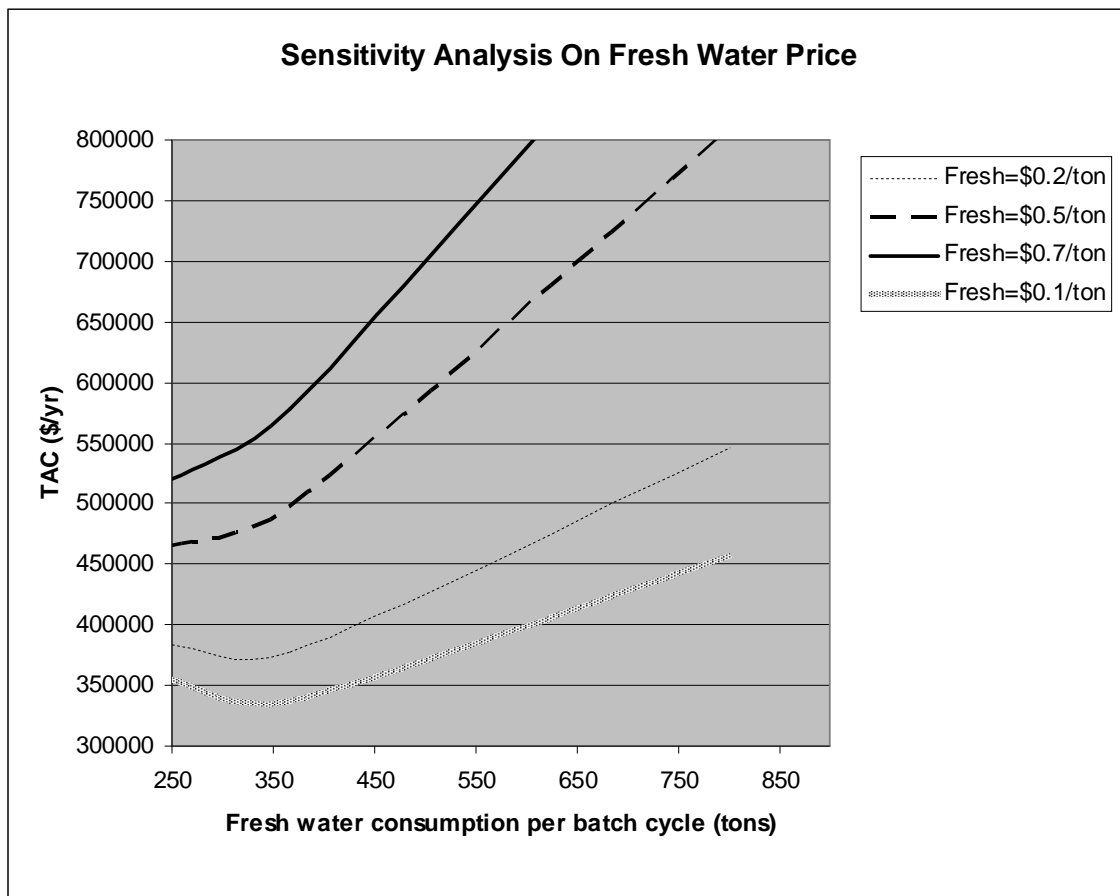


Fig. 3.4. Sensitivity Analysis on Fresh Water Cost

### 3.6 Summary

This work has developed a novel systematic procedure to synthesize and schedule a cost effective batch water network. In addition to sources and sinks, two sets of tanks have been introduced for storage and dispatch. This new arrangement overcomes previous-research limitations that restricted assignment within the same batch cycle and were not capable of insuring sink feasibility when supply and demand overlap. The first step in the procedure determines water targets for both fresh water and wastewater by developing a representation with no scheduling limitations. This representation involves the use of infinite tanks which has been mathematically transformed into direct assignment of sources to sinks. Next, the problem of determining the minimum fixed cost or the minimum number of tanks has been formulated. Finally, an iterative procedure has been established to trade off operating and fixed costs (e.g., by iteratively trading off fresh water consumption and number of tanks) until the minimum TAC is identified.

## **CHAPTER IV**

### **SYNTHESIS AND SCHEDULING OF BATCH WATER-RECYCLE NETWORKS WITH STORAGE AND DISPATCH**

#### **4.1 Introduction**

Industries around the world are seeking efficient methods to conserve natural resources. Consequently, there is an ongoing drive towards increasing the utilization of process resources to decrease consumption of external resources. One of the most widely and extensively used resources in industry is water. In addition to its impact on natural resources and cost, excessive usage of water also leads to the discharge of significant quantities of wastewater. Consequently, responsible industries have begun to take considerable actions to identify ways to reduce fresh water consumption and wastewater generation. One effective approach has been to maximizing water reuse and recycle within the process plant. The numerous water sources and users must be simultaneously addressed. This leads to the need for efficient techniques to design water recycle networks to optimize the use of fresh water, recycle of process water, and discharge of wastewater.

Recently, significant contributions have been made in developing systematic techniques for the synthesis of industrial water networks. To date, the majority of the water-

network research has focused on continuous, steady-state processes. Recent reviews of steady-state water networks can be found in literature (e.g., El-Halwagi, 2006; El-Halwagi et al., 2003; Mann and Liu, 2000; Bagajewicz, 2000). Much less attention has been given to batch water processes. Given that batch systems are common within industry, it is important to develop batch water recycle networks that minimize fresh water consumption, and wastewater discharge.

Wang and Smith, 1995, developed a time-pinch analysis method which uses graphical techniques to synthesize batch water networks. This technique treats time as the primary constraint and concentration as the secondary constraint. Majozi et al., 2006, also devised a graphical technique which is an extension of the time-pinch analysis technique. Both of these techniques were limited to water-using units that are modeled as mass exchangers and deal with single-contaminant systems. Foo et al., 2005, devised a graphical method known as water cascade analysis which is limited to single contaminant systems. Also, mixing of water sources at different impurities in the same tank was not allowed. Kim and Smith, 2004, and Majozi, 2005a, b, developed mathematical formulations that optimize water usage and network configuration. These formulations are limited to mass transfer based water units and single contaminant systems. Chang and Li, 2006, also developed a mathematical formulation for batch networks that are not limited to mass transfer based water units.

The previous research efforts have provided valuable tools and insights for batch water-network design. Nonetheless, they suffer from one or more of the following assumptions and limitations:

- **Recycle within the same cycle:** According to this assumption, water recycle is limited to units that require water later in the same cycle (i.e., no recycle from one batch cycle to another). In many cases, it may be beneficial to recycle water from a source which is available later in a cycle to a user which demands water earlier in the cycle. This can be achieved by storing water from one cycle and using it in another cycle.
- **Lumped usage of water over a cycle:** This assumption accounts for a total quantity and quality of water supply and demand. Such an assumption can lead to wrong results when the demand overlaps with the supply. As an illustration, consider the case shown by Fig. 4.1 with two water sources that are mixed and recycled to a water-demanding unit. Suppose that the first source is available from time  $t_1$  to  $t_3$  while the second source is available from time  $t_2$  to  $t_5$ . The quantities and compositions for sources I and II are given by  $W_I$ ,  $W_{II}$ ,  $y_I$ , and  $y_{II}$ , respectively. The sink demands a total quantity of  $W_I + W_{II}$  of water. The maximum admissible composition to the sink is given by:

$$Z^{\max} = \frac{W_I y_I + W_{II} y_{II}}{W_I + W_{II}} \quad (4.1)$$

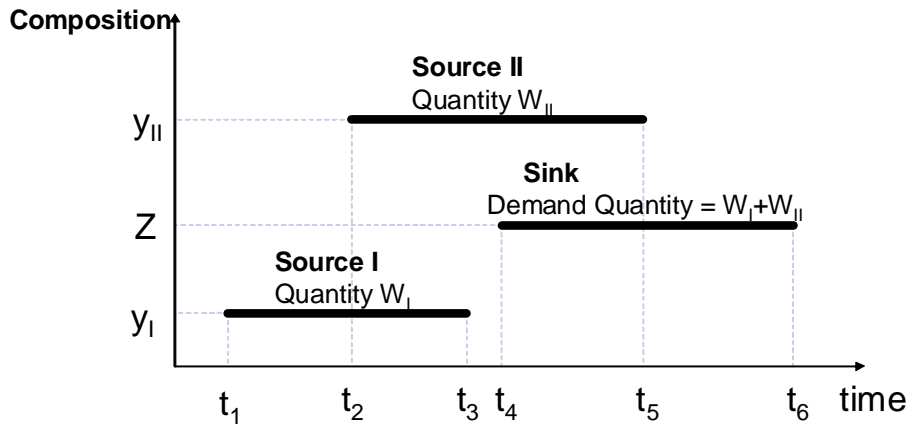


Fig. 4.1. Illustrating Example for Limitation of Averaging Supply

The two sources may be stored in a tank and used to provide feed to the sink. On a cycle basis, the stored mixture satisfies the sinks demand for water quantity and composition. However, there is a problem with implementation. When the sink begins to draw water at time  $t_4$ , the composition of the stored mixture (of the whole of source I and the quantity of source II generated from  $t_2$  to  $t_4$ ), will initially be satisfactory since it is less than  $Z^{max}$ . However, as time progresses the concentration of the mixture will continually increase (since only higher-composition source II is contributing to the storage tank). Therefore, before reaching  $t_6$ , the stored mixture will have a composition exceeding  $Z^{max}$ . Since cycle-based averages do not capture such violation, this example underscores the need for detailed scheduling.

- Fresh-water minimization: The overwhelming majority of research on water-recycle networks has focused on the objective of minimizing fresh water usage and wastewater discharge. While this is a useful objective from an operating-cost perspective, it is also important to consider a more comprehensive objective dealing with the fixed cost in addition to the operating cost.

The objective of this research is to develop a systematic procedure to synthesize and schedule a cost effective batch water network, while meeting all process constraints. The aforementioned limitations of previous research efforts are overcome. A source-tank-sink structural representation is developed to account for the potential configurations of the water network. This representation allows for separate tanks to be used for storage and dispatch over alternating cycles. A mathematical formulation is developed to solve the problem by minimizing the total annualized cost (TAC) while determining sufficient information on the design and scheduling of the network. The items which dominate the fixed cost of the network are the storage and dispatch tanks and the piping that connects the sources, tanks, and sinks. The items which dominate the operating cost are the fresh water and waste water treatment. Next, simplification of the network is done by following guidelines introduced to the designer. Additionally, further analysis may be made by implementing integer cut constraints on tanks in order to evaluate different network configurations and schedules. A case study is solved to illustrate the merits of the developed approach.



## 4.2 Nomenclature

Before proceeding to the problem statement and approach, it is useful to introduce the various symbols used throughout this work:

### *Indices*

$d$	Single tank dispatching at one time interval
$h$	Fresh water stream
$p$	Pair of double tanks
$q$	Discretization index for time intervals
$r$	Single tank receiving at one time interval
$s$	Sinks
$t$	Time
$\tau$	Cycle time
$u$	Impurity component
$v$	Sources

### *Sets*

$DSTANKS$	Set of single tanks delivering in interval $q$
$DTANKS$	Set of double tanks
$RSTANKS$	Set of single tanks receiving in interval $q$
$SINKS$	Set of process sinks

$SINK_{sq}$	Set of process sinks demanding water at time interval $q$
$SOURCES$	Set of process sources
$SOURCE_{sq}$	Set of process sources available at time interval $q$

### *Parameters*

$a_{structural}$	Cost coefficient for the structural cost of pipelines
$b$	Cost coefficient related to the capacity of pipelines
$c$	Cost coefficient related to the capacity of pipelines
$Cost_{DT}$	Cost of double tanks $p$
$Cost_{fresh}$	Cost of fresh water stream $h$
$Cost_{ST}$	Cost of single tank
$Cost_{waste}$	Cost of waste water treatment
$G_{s,q}$	Water demand of sink $s$ over period $q$
$J$	Upper bound on maximum capacity of pipelines
$N_{SK}$	Number of process sinks
$N_{SR}$	Number of process sources
$N_t$	Number of multiple time periods per cycle
$U$	Upper bound on maximum capacity of tank
$W_{v,q}$	Amounts of source $v$ over period $q$

$x_{h,u}$	Composition of component $u$ in fresh water stream $h$
$y_{v,q,u}$	Composition of component $u$ in source $v$ over period $q$
$Z_{s,q,u}^{\max}$	Maximum admissible composition of component $u$ to sink $s$ over period $q$

### Variables

$C_{q,d_q}^{ST, Dispatching\ q}$	Capacity of single tank $d_q$
$C_{q,r_q}^{ST, Storing\ q}$	Capacity of single tank $r_q$
$C_p^{DT}$	Capacity of double tank $p$
$DT_p$	Zero/one binary integer variable designating the absence/existence of double tank $p$
$Fresh$	Total quantity of fresh water consumption per batch cycle
$I_{d_q,s,q}$	Zero/one binary integer variable designating the absence/existence of piping to connect tank $d_q$ to sink $s$
$I_{p,s,q}$	Zero/one binary integer variable designating the absence/existence of piping to connect tank $p$ to sink $s$
$I_{r_q,s,q'}$	Zero/one binary integer variable designating the absence/existence of piping to connect tank $r_q$ to sink $s$
$I_{v,q,d_q}$	Zero/one binary integer variable designating the absence/existence of piping to connect source $v$ to tank $d_q$

$I_{v,q,p}$	Zero/one binary integer variable designating the absence/existence of piping to connect source $v$ to tank $p$
$I_{v,q,r_q}$	Zero/one binary integer variable designating the absence/existence of piping to connect source $v$ to tank $r_q$
$I_{v,q,waste}$	Zero/one binary integer variable designating the absence/existence of piping to connect source $v$ to waste
$ST_{q,d_q}^{Dispatching\ q}$	Zero/one binary integer variable designating the absence/existence of single tank $d_q$
$ST_{q,r_q}^{Storing\ q}$	Zero/one binary integer variable designating the absence/existence of single tank $r_q$
$t_{d_q,s,q}^{ST,Dispatching\ q}$	Amount of water from single tank $d_q$ dispatched to sink $s$ over period $q$
$t_{p,s,q}^{DT}$	Amount of water from double tank $p$ dispatched to sink $s$ over period $q$
$t_{r_q,s,q}^{ST,Storing\ q}$	Amount of water from single tank $r_q$ dispatched to sink $s$ over period $q$
$Waste$	Total quantity of source water dispatched to waste per batch cycle
$W_{v,q}^{Direct}$	Amounts of source $v$ over period $q$ that is assigned directly to sinks
$W_{v,q}^{DT}$	Amounts of source $v$ over period $q$ that is assigned to double tanks
$W_{v,q}^{ST}$	Amounts of source $v$ over period $q$ that is assigned to a single tank
$w_{v,q,s}^{Direct}$	Amounts of source $v$ over period $q$ that is assigned directly to sink $s$
$w_{v,q,d_q}^{ST,Dispatching\ q}$	Amounts of source $v$ over period $q$ that is assigned to single tank $d_q$
$w_{v,q,p}^{DT}$	Amounts of source $v$ over period $q$ that is assigned to double tank $p$
$w_{v,q,r_q}^{ST,Storing\ q}$	Amounts of source $v$ over period $q$ that is assigned to single tank $r_q$
$W_{v,q,waste}$	Amounts of source $v$ over period $q$ that is assigned to waste

$y_{d_q,u}^{ST,Dispatching\_q}$	Composition of impurity $u$ in single tank $d_q$
$y_{p,u}^{DT}$	Composition of impurity $u$ in double tank $p$
$y_{r_q,u}^{ST,Storing\_q}$	Composition of impurity $u$ in single tank $r_q$
$Z_{s,q,u}$	Composition of impurity $u$ dispatched to sink $s$ over period $q$

### 4.3 Problem Statement

The batch water network problem to be addressed in this work may be stated as follows:

During a batch process with a given cycle time ( $\tau$ ), there are a number of water sources and sinks characterized by the following:

- Sources: There is a set  $SOURCES = \{v|v=1,2,\dots, N_{SR}\}$  of process water streams. The dynamic profiles for the flow rate and composition of each source,  $v$ , are known and given by  $w_v(t)$  and  $y_{v,u}(t)$  where  $u$  is an index for components and  $t$  is the time from the beginning of the cycle ( $0 \leq t \leq \tau$ ).
- Sinks: There is a set  $SINKS = \{s|s=1,2,\dots, N_{SK}\}$  of process units that require water. Constraints on dynamic profiles for the flow rate and maximum admissible composition of impurity of each sink  $s$  are known and given by  $g_s(t)$  and  $z_{s,u}^{\max}(t)$ .

Available for service are:

- A number of fresh water streams; each fresh stream  $h$  has a given concentration of the  $u^{\text{th}}$  impurity designated by  $x_{h,u}$ .

It is desired to develop a systematic procedure to synthesize and schedule a batch water network in which water from sources may be stored in tanks then recycled to sinks when needed or released as waste. The water network must be cost effective and meet all process constraints. The synthesis and scheduling tasks require the identification of the following:

- What is the optimum network configuration including assignment of sources and sinks?
- Which fresh stream(s) should be used? How much of each?
- How many tanks should be used? What are their sizes? What are their feeds?
- How should the synthesized network be scheduled for operation?

#### **4.4 Approach**

The following elements will be used in the approach to synthesize a cost effective batch water network:

1. Multi-period reformulation of the continuous sources and sinks
2. Development of a structural representation to embed network configurations of interest for design and scheduling (including storage and dispatch between each two subsequent cycles)
3. Development and solution of a mathematical formulation which is aimed at minimizing the total annualized cost of the network while determining key design and scheduling information.

4. Inspect Network for tank simplification.
5. Addition of integer cut constraints on tanks to generate alternative network configurations.

#### 4.4.1 Multi-Period Reformulation of Sources and Sinks

Due to the dynamic variation of both the sources and the sinks, it is more convenient to transform the problem data and constraints into discrete sets. This is achieved by invoking a multi-period reformulation where the process sources and the sink constraints are discretized over time intervals. The cycle time is discretized into a number  $N_t$  of time intervals. These time intervals are selected to be large enough to capture significant changes in composition for the sources or meaningful changes in the constraints for the sinks. The discretization index is referred to as  $q$ . The  $q^{\text{th}}$  time interval between indices  $q-1$  and  $q$  is described by the following time interval  $[t_{q-1}$  and  $t_q]$ . For the sources, the time domain is decomposed into  $N_t$  time intervals. The flow rate profile of each source,  $v$ , is transformed into a discrete set of flows per cycle (water quantities per cycle not continuous flow rates). For the  $q^{\text{th}}$  time interval, the quantity of the  $v^{\text{th}}$  source is given by:

$$W_{v,q} = \int_{t_{q-1}}^{t_q} w_v(t) dt \quad (4.2)$$

and the composition of the pollutant is given by:

$$y_{v,q} = \frac{\int_{t_{q-1}}^{t_q} w_v(t) y_v(t) dt}{W_{v,q}} \quad (4.3)$$

Similarly, for the sinks, the time domain is decomposed into  $N_t$  time intervals with the multiperiod index  $q$  used for discretization to define the time interval  $[t_{q-1}$  and  $t_q]$ . The constraint for flow rate profile of each sink,  $s$ , is transformed into a discrete set of constraints on flows as follows:

$$G_{s,q} = \int_{t_{q-1}}^{t_q} g_s(t) dt \quad (4.4)$$

and the composition constraints of the pollutant are given by:

$$z_{s,q}^{\max} = \frac{\int_{t_{q-1}}^{t_q} g_s(t) z_s^{\max}(t) dt}{G_{s,q}} \quad (4.5)$$

The foregoing discretization and reformulation are carried out as a pre-synthesis task. Therefore, the problem formulation will involve multi-period algebraic equations instead of the simultaneous algebraic and differential equations.



#### 4.4.2 Structural Representation

The next step in designing a batch water network is developing a structural representation which embeds all potential configurations of the network and enables proper scheduling. As mentioned before, earlier approaches have been restricted by two scheduling limitations: recycle within the same cycle and lumped usage of water over a cycle. These limitations can be overcome. Therefore, the following three scenarios are envisioned:

1. **Direct assignment of sources to sinks:** For a sink  $s$  which corresponds to time interval  $q$ , the sources available over the same time interval may be directly assigned to the sink without the need for storage or dispatch tanks. The flow of each source to be assigned to the sink is unknown and is to be determined through optimization. Fig. 4.2 is a representation of directly assigning the sources to sinks during the same time interval.

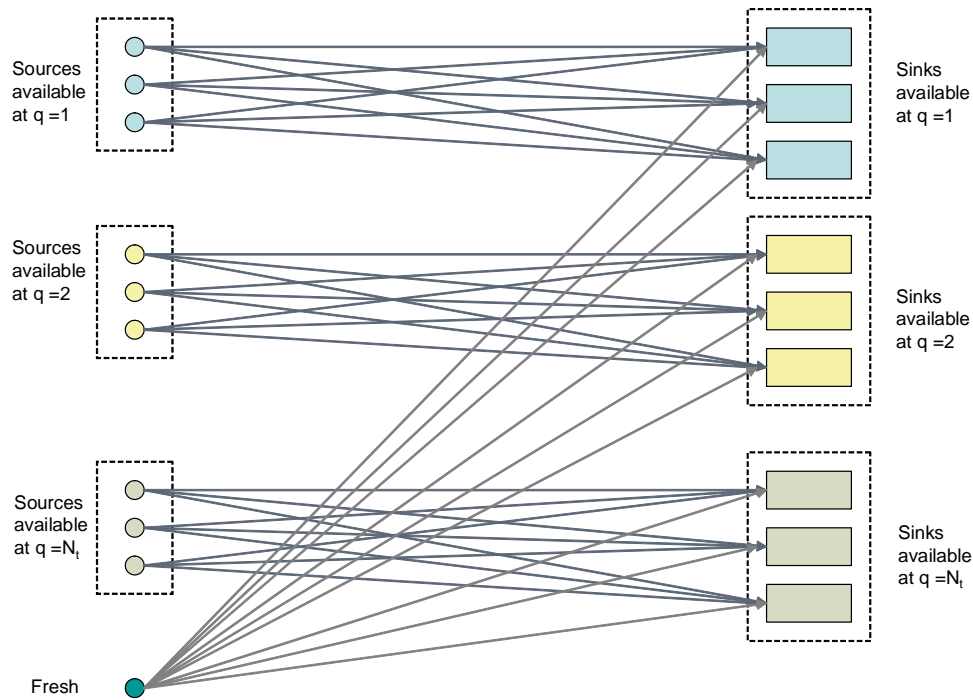


Fig. 4.2. Source-Sink Direct Assignment

2. **Assignment of sources to single tanks:** As shown by Fig. 4.1 and the associated discussion, it is possible to use a single set of tanks (each of which serving the dual purposes of storage and dispatch) unless storage and dispatch occur over the same time interval. This is attributed to the observation from Fig. 4.1. Suppose that the tank has already stored water from sources available at times  $q' \neq q$ . When a source is fed to the tank during period  $q$  while the tank is dispatching water within the same interval, the composition within the tank will change over period  $q$  and will

not meet the optimal composition fed to the sink throughout period  $q$ . Therefore, two scenarios are considered:

- a. A tank storing at intervals  $q' \neq q$  and dispatching at interval  $q$ :** Consider a sink that operates over period  $q$ . Sources existing over all other time intervals (excluding period  $q$ ) may be stored in a tank. The stored water is dispatched to the sink during period  $q$ . Therefore, the single tank serves both purposes of storage and dispatch. It is worth noting that any source that belongs to  $SOURCES_q$  is excluded from this arrangement. Another observation is that  $q'$  does not have to be less than  $q$ . Indeed, a sink operating at period  $q$  may receive water from a tank that has been fed by sources in intervals before  $q$  (within the same cycle) or after  $q$  (from the previous cycle). Aside from the startup during the first cycle, this arrangement will work properly for the remaining cycles. This arrangement is shown in Fig. 4.3a. The illustration is shown for tanks collecting at any time interval except  $q = 1$  and dispatching during period  $q = 1$ . Therefore, a set of single tanks are defined to dispatch at interval  $q$  while collecting from sources at time periods excluding interval  $q$ . This set of single tanks dispatching in interval  $q$  is defined as  $DSTANKS = \{d_q | d_q = 1, 2, \dots, N_{Dispatching\ ST, q}\}$ . The capacity of the  $d_q^{th}$  tank is given by:

$$C_{q, d_q}^{ST, Dispatching\ q} = \sum_{\substack{v \in SOURCES_{q'} \\ \forall q', q' \neq q}} w_{v, q', d_q}^{ST, Dispatching\ q} \quad \forall q, d_q \quad (4.6)$$

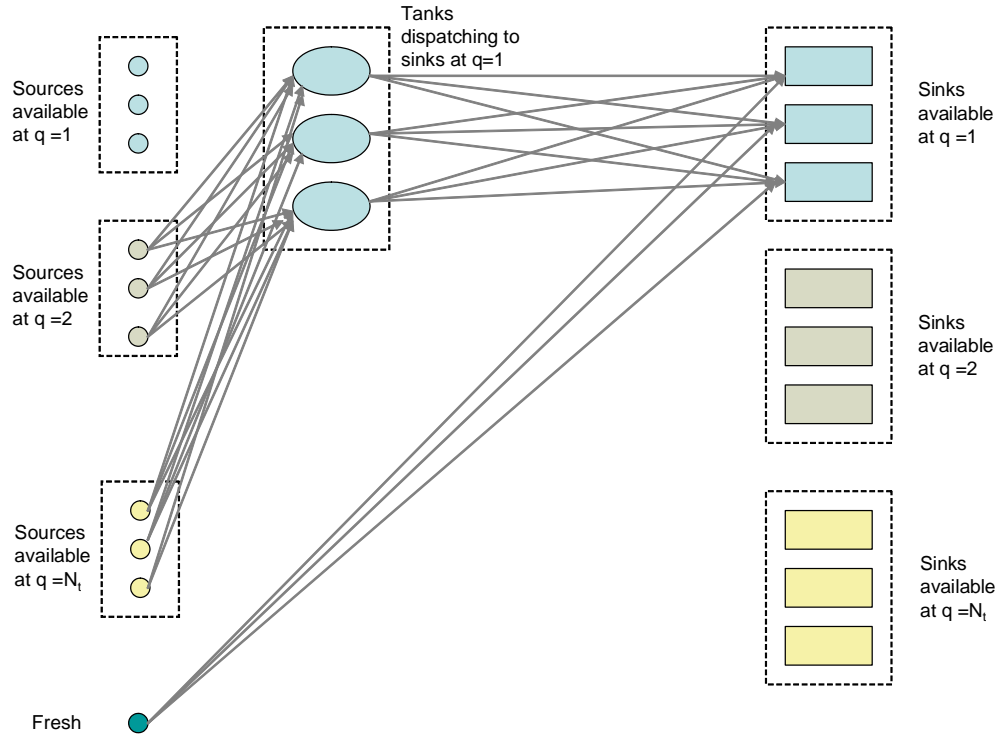


Fig. 4.3a. Assignment to Single Tanks Receiving from Different Periods and Delivering to a Single Period

The presence or absence of each of these tanks is determined by a binary integer variable  $ST_{q,d_q}^{Dispatching\ q}$  whose value may be determined through the following constraint:

$$C_{q,d_q}^{ST, Dispatching\ q} \leq ST_{q,d_q}^{Dispatching\ q} * U \quad \forall q, d_q \quad (4.7)$$

$U$  is a sufficiently large number (e.g., maximum allowable capacity of a tank).

- b. A tank storing at interval  $q$  and dispatching to sinks at intervals  $q' \neq q$ :** In this scenario, a set of tanks are designated for each time interval  $q$ . Each of these tanks collects from sources that belong to  $SOURCES_q$  and dispatch to  $SINKS_{q'}$  where  $q' \neq q$ . This scenario is illustrated by Fig. 4.3b for the case when the tanks collect water during  $q = 1$  and deliver water to sinks in subsequent intervals. Therefore, a set of single tanks are defined to store from sources at interval  $q$  while dispatching to sinks at time periods excluding interval  $q$ . This set of single tanks receiving in interval  $q$  is defined as  $RSTANKS = \{r_q | r_q = 1, 2, \dots, N_{Receiving\ ST, q}\}$ . The capacity of the  $r_q^{th}$  tank is given by:

$$C_{q,r_q}^{ST, Storing\ q} = \sum_{v \in SOURCES_q} w_{v,q,r_q}^{ST, Storing\ q} \quad \forall q, r_q \quad (4.8)$$

The presence or absence of each of these tanks is determined by a binary integer variable  $ST_{q,r_q}^{Storing\ q}$  whose value may be determined through the following constraint:

$$C_{q,r_q}^{ST, Storing\ q} \leq ST_{q,r_q}^{Storing\ q} * U \quad \forall q, r_q \quad (4.9)$$

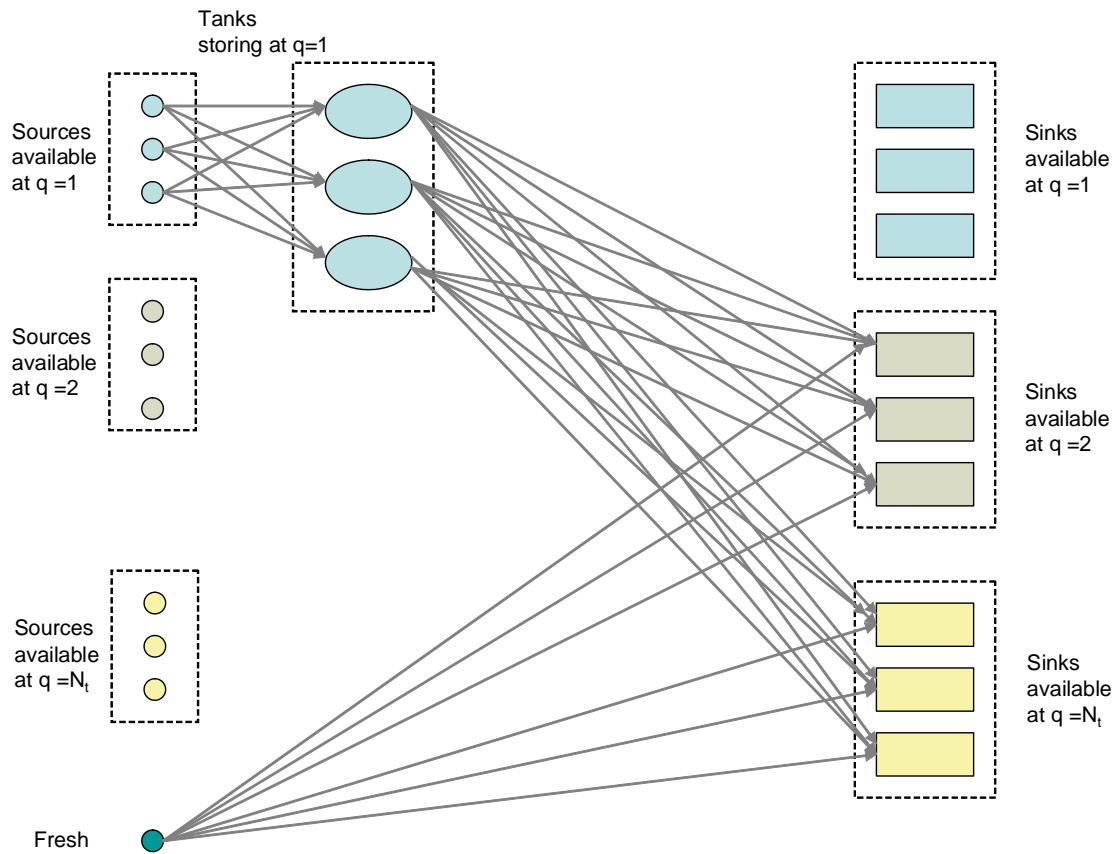


Fig. 4.3b. Assignment to Single Tanks Receiving from a Single Period and Delivering to Multiple Periods

3. **Assignment of sources to two tanks:** In this case, two sets of tanks are used: one set for storage and another for dispatch. Every cycle, the role of each set of tanks alternates. Therefore, during one cycle, the storage tanks will be collecting water from sources and in the next cycle, these tanks will be used to dispatch the stored

water to the sinks. Consider a sink that operates over period  $q$ . Sources existing over all time intervals (including period  $q$ ) may be stored in a tank. As shown by Fig. 4.1, two tanks are needed to insure proper scheduling: while one tank stores water, the other tank is used to dispatch water. In the subsequent cycle, the roles of the tanks are switched such that the dispatch tank is used for storage while the tank that previously stored water is used for dispatch. The storage-dispatch arrangement also insures proper satisfaction of sink constraints even when source supply and sink demand overlap (as shown by Fig. 4.1). The double-tank arrangement is shown in Fig. 4.4. The following set of double tanks is defined:  $DTANKS = \{p | p = 1, 2, \dots, N_{DT}\}$ . The capacity of the  $p^{th}$  tank is given by:

$$C_p^{DT} = \sum_{\substack{v \in SOURCES_q \\ \forall q}} w_{v,q,p}^{DT} \quad \forall p \quad (4.10)$$

The presence or absence of each of these tanks is determined by a binary integer variable  $DT_p$  whose value may be determined through the following constraint:

$$C_p^{DT} \leq DT_p * U \quad \forall p \quad (4.11)$$

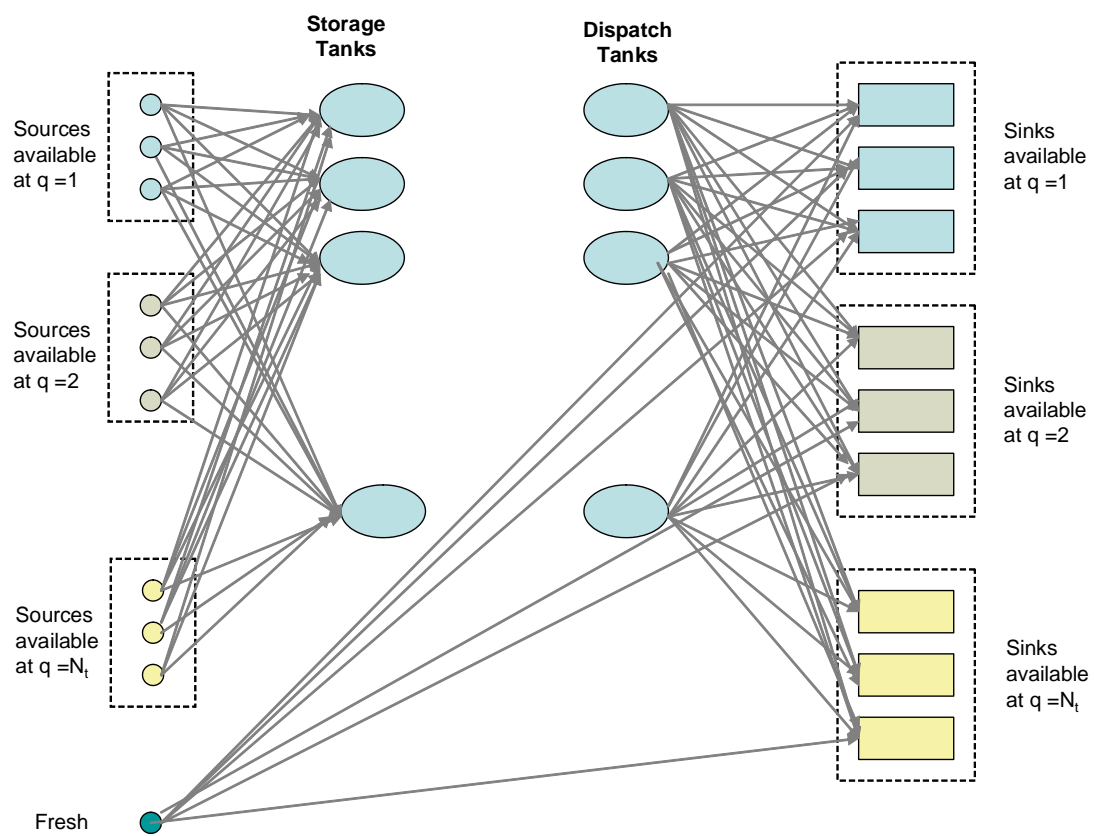


Fig. 4.4. Double Sets of Tanks for Storage and Dispatch



4. **Assignment of sources to waste:** Sources that are not assigned to sinks or tanks are discharged as waste.

Based on the foregoing discussion, Fig. 4.5 is a structural representation of the configurations of interest. Each source is split into several fractions. These fractions are assigned directly to sinks, to single tanks, to two tanks, and to waste. The guidelines for assigning sources to sinks or tanks follow the aforementioned rules. The unallocated sources are discharged to waste.

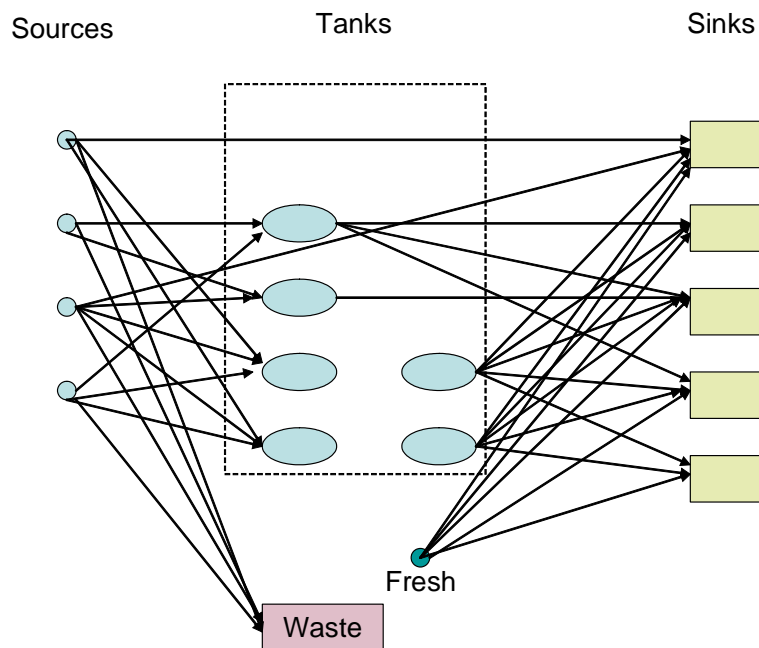


Fig. 4.5. Source-Tank-Sink Representation with Direct Assignment, Single Tanks, and Double Tanks for Storage and Dispatch

#### 4.4.3 Mathematical Formulation

The next step is to formulate an optimization program whose solution will provide sufficient information to synthesize and schedule a cost effective batch water network while still meeting all process constraints. In the objective function, both fixed and operating costs are involved in calculating in the total annualized cost (TAC). The items which dominate the fixed cost are the storage and dispatch tanks and the piping and pumping system for connecting the sources, the tanks, and the sinks. The items which dominate the operating cost are the expenses associated with the supply of fresh water and the treatment of wastewater. Therefore, the objective function is expressed as follows:

Minimize TAC =

$$\begin{aligned}
 & Cost_{ST} \left( \sum_{\forall q} C_{q,d_q}^{ST, Dispatching\_q} + \sum_{\forall q} C_{q,r_q}^{ST, Storing\_q} \right) + Cost_{DT} \sum_{\forall p} C_p^{DT} + Cost_{fresh} Fresh + Cost_{waste} Waste \\
 & + \sum_{\forall v} \sum_{\forall q} \sum_{\forall s} (a_{structural} + b * Capacity^c) I_{v,q,s} + \sum_{\forall v} \sum_{\forall q} \sum_{\forall r_q} (a_{structural} + b * Capacity^c) I_{v,q,r_q} \\
 & + \sum_{\forall v} \sum_{\forall q} \sum_{\forall d_q, d_q \neq q} (a_{structural} + b * Capacity^c) I_{v,q,d_q} + \sum_{\forall v} \sum_{\forall q} \sum_{\forall p} (a_{structural} + b * Capacity^c) I_{v,q,p} \\
 & + \sum_{\forall r_q} \sum_{\forall s} \sum_{\forall d_q, d_q \neq q} (a_{structural} + b * Capacity^c) I_{r_q,s,d_q} + \sum_{\forall d_q} \sum_{\forall s} \sum_{\forall q} (a_{structural} + b * Capacity^c) I_{d_q,s,q} \\
 & + \sum_{\forall p} \sum_{\forall s} \sum_{\forall q} (a_{structural} + b * Capacity^c) I_{p,s,q} + \sum_{\forall v} \sum_{\forall q} (a_{structural} + b * Capacity^c) I_{v,q,waste}
 \end{aligned} \tag{4.12}$$

where  $Cost_{ST}$ ,  $Cost_{DT}$ ,  $Cost_{fresh}$ , and  $Cost_{waste}$  are the cost coefficients for single tanks, double tanks, fresh water, and waste water treatment respectively. Also,  $(a_{structural} + b * Capacity^c)$  is the cost function for the needed piping to dispatch source water to sinks directly, source water to single tanks, source water to double tanks, source water to waste, and stored water to sinks. The cost coefficient  $a_{structural}$  takes into account the structural cost to implement the needed piping. Coefficients  $b$  and  $c$  take into account the cost associated with the capacity of the piping.  $I_{v,q,s}$ ,  $I_{v,q,r_q}$ ,  $I_{v,q,d_q}$ ,  $I_{v,q,p}$ ,  $I_{v,q,waste}$ ,  $I_{r_q,s,q}$ ,  $I_{d_q,s,q}$ , and  $I_{p,s,q}$  are binary integers designating the existence or absence of piping used for dispatching sources to sinks, sources to single tanks  $r_q$ , sources to single tanks  $d_q$ , sources to a double tank configuration, sources to waste, stored water in tank  $r_q$  to sinks, stored water in tank  $d_q$  to sinks, and stored water in a double tank configuration to sinks.

The following constraints are used:

Splitting of Sources:

$$W_{v,q} = W_{v,q}^{Direct} + W_{v,q}^{ST} + W_{v,q}^{DT} + W_{v,q,waste} \quad (4.13)$$

where  $W_{v,q}^{Direct}$ ,  $W_{v,q}^{ST}$ ,  $W_{v,q}^{DT}$ , and  $W_{v,q,waste}$  are the amounts of source  $v$  over period  $q$  that are respectively assigned directly to sinks, to single tanks (that serves both tasks of

storage and dispatch), to two tanks (storage and dispatch), and to waste. Fig. 4.6 is a representation of the water balance for splitting a source. The following expressions are used for the water-balance terms:

Direct assignment of sources to sinks within the same time interval:

$$W_{v,q}^{Direct} = \sum_{s \in SINKS_q} w_{v,q,s}^{Direct} \quad \forall v, q \quad (4.14)$$

where  $\sum_{s \in SINKS_q} w_{v,q,s}^{Direct}$  is the sum of the source water directly assigned to sinks,

Assignment of sources to single tanks:

$$W_{v,q}^{ST} = \sum_{r_q \in RSTANKS_q} w_{v,q,r_q}^{ST, Storing\ q} + \sum_{\substack{d_{q'} \in DSTANKS_{q'} \\ \forall d_{q'}, q' \neq q}} w_{v,q,d_{q'}}^{ST, Dispatching\ q} \quad \forall v, q \quad (4.15)$$

where  $\sum_{r_q \in RSTANKS_q} w_{v,q,r_q}^{ST, Storing\ q}$  is the sum of the source water  $v$  over period  $q$  assigned to single

tanks receiving at one time interval  $q$ , and  $\sum_{\substack{d_{q'} \in DSTANKS_{q'} \\ \forall d_{q'}, q' \neq q}} w_{v,q,d_{q'}}^{ST, Dispatching\ q}$  is the sum of the source

water  $v$  over period  $q$  assigned to single tanks delivering water at one time interval  $q'$ ,

Assignment of sources to double tanks:

$$W_{v,q}^{DT} = \sum_{p \in DTANKS} w_{v,q,p}^{DT} \quad \forall v, q \quad (4.16)$$

where  $\sum_{p \in DTANKS} w_{v,q,p}^{DT}$  is the sum of the source water  $v$  over period  $q$  assigned to double tanks.

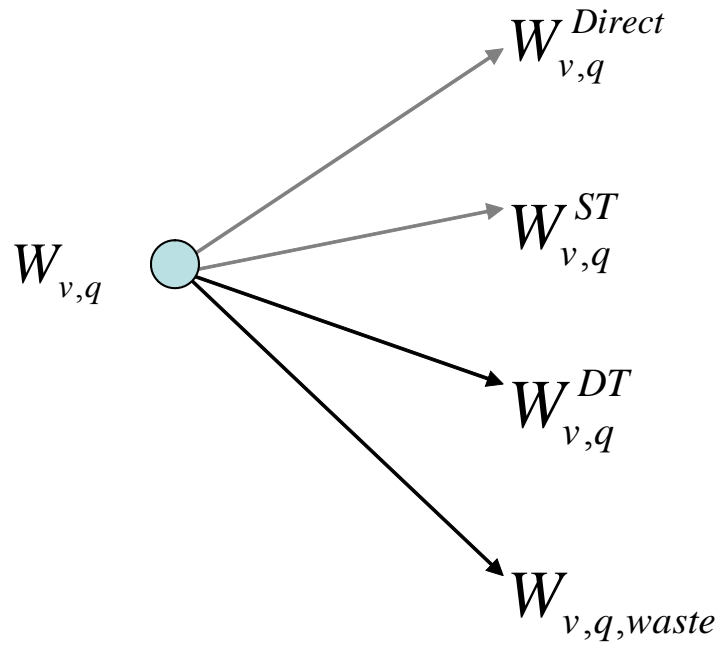


Fig. 4.6. Water Balance for Splitting a Source

Single-Tank Balances, Capacities, and Existence:

$$C_{q,d_q}^{ST, Dispatching\ q} = \sum_{\substack{v \in SOURCES_{q'} \\ \forall q', q' \neq q}} w_{v,q',d_q}^{ST, Dispatching\ q} \quad \forall q, d_q \quad (4.17)$$

where  $C_{q,d_q}^{ST, Dispatching\ q}$  is the capacity of single tank  $d_q$ ,

$$C_{q,d_q}^{ST, Dispatching\ q} * y_{d_q,u}^{ST, Dispatching\ -q} = \sum_{\substack{v \in SOURCES_{q'} \\ \forall q', q' \neq q}} w_{v,q',d_q}^{ST, Dispatching\ q} * y_{v,q',u} \quad \forall q, d_q, u \quad (4.18)$$

where  $y_{d_q,u}^{ST, Dispatching\ -q}$  is the composition of the stored water in single tank  $d_q$ , and  $y_{v,q',u}$

is the composition of source  $v$  over period  $q'$  assigned to single tank  $d_q$ ,

$$C_{q,d_q}^{ST, Dispatching\ q} \leq ST_{q,d_q}^{Dispatching\ q} * U \quad \forall q, d_q \quad (4.19)$$

where  $ST_{q,d_q}^{Dispatching\ q}$  is a zero/one binary integer variable designating the

absence/existence of single tank  $C_{q,d_q}^{ST, Dispatching\ q}$ , and  $U$  is the upper capacity of the tank,

The following constraints are used:

$$C_{q,d_q}^{ST, Dispatching\ q} = \sum_{\forall s} \sum_{\forall q' = q} t_{d_q,s,q'}^{ST, Dispatching\ q} \quad \forall q, d_q \quad (4.20)$$

where  $t_{d_q, s, q}^{ST, Dispatching\ q}$  is the quantity of stored source water from tank  $d_q$  assigned to sink  $s$  over time interval  $q$

$$C_{q, r_q}^{ST, Storing\ q} = \sum_{v \in SOURCES_q} w_{v, q, r_q}^{ST, Storing\ q} \quad \forall q, r_q \quad (4.21)$$

where  $C_{q, r_q}^{ST, Storing\ q}$  is the capacity of single tank  $r_q$ ,

$$C_{q, r_q}^{ST, Storing\ q} * y_{r_q, u}^{ST, Storing\ q} = \sum_{v \in SOURCES_q} w_{v, q, r_q}^{ST, Storing\ q} * y_{v, q, u} \quad \forall q, r_q, u \quad (4.22)$$

where  $y_{r_q, u}^{ST, Storing\ q}$  is the composition of the stored water in single tank  $r_q$ , and  $y_{v, q, u}$  is the composition of source  $v$  over period  $q$  assigned to single tank  $r_q$ ,

$$C_{q, r_q}^{ST, Storing\ q} \leq ST_{q, r_q}^{Storing\ q} * U \quad \forall q, r_q \quad (4.23)$$

where  $ST_{q, r_q}^{Storing\ q}$  is a zero/one binary integer variable designating the absence/existence of single tank  $C_{q, r_q}^{ST, Storing\ q}$ , and  $U$  is the upper capacity of the tank,

$$C_{q, r_q}^{ST, Storing\ q} = \sum_{\forall s} \sum_{\forall q' \neq q} t_{r_q, s, q'}^{ST, Storing\ q} \quad \forall q, r_q \quad (4.24)$$

where  $t_{r_q, s, q'}^{ST, Storing\ q}$  is the quantity of stored source water from tank  $r_q$  assigned to sink  $s$  over time interval  $q'$ ,

Double-Tank Balances, Capacities, and Existence:

$$C_p^{DT} = \sum_{\substack{v \in SOURCESq \\ \forall q}} w_{v,q,p}^{DT} \quad \forall p \quad (4.25)$$

where  $C_p^{DT}$  is the capacity of one of the double tanks  $p$ ,

$$C_p^{DT} * y_{p,u}^{DT} = \sum_{\substack{v \in SOURCESq \\ \forall q}} w_{v,q,p}^{DT} * y_{v,q,u} \quad \forall p, u \quad (4.26)$$

where  $y_{p,u}^{DT}$  is the composition of the stored water in double tanks  $p$ , and  $y_{v,q,u}$  is the composition of source  $v$  over period  $q$  assigned to double tanks  $p$ ,

$$C_p^{DT} \leq DT_p * U \quad \forall p \quad (4.27)$$



where  $DT_p$  is a zero/one binary integer variable designating the absence/existence of the double tank, and  $U$  is the upper capacity of tank  $C_p^{DT}$  in the double tank arrangement,

$$C_p^{DT} = \sum_{\forall s} \sum_{\forall q} t_{p,s,q}^{DT} \quad \forall p \quad (4.28)$$

where  $t_{p,s,q}^{DT}$  is the quantity of stored source water from tanks  $p$  assigned to sink  $s$  over time interval  $q$ .

Waste flow:

$$Waste = \sum_v \sum_q W_{v,q,waste} \quad (4.29)$$

where  $W_{v,q,waste}$  is the quantity of source  $v$  over period  $q$  dispatched to waste,

Sink balances:

$$G_{s,q} = \sum_{\forall q'=q} t_{d_{q'},s,q}^{ST,Dispatching-q'} + \sum_{\forall q' \neq q} t_{r_{q'},s,q}^{ST,Storing-q'} + \sum_{\forall p} t_{p,s,q}^{DT} + \sum_{\forall h} f_{h,s,q} \quad \forall q,s \quad (4.30)$$

where  $t_{d_{q'},s,q}^{ST,Dispatching-q'}$ ,  $t_{r_{q'},s,q}^{ST,Storing-q'}$ ,  $t_{p,s,q}^{DT}$  and  $f_{h,s,q}$  are stored source water from tanks and fresh water that is assigned to sink s in time interval q,

$$G_{s,q} * Z_{s,q,u} = \sum_{\forall q'=q} t_{d_{q'},s,q}^{ST,Dispatching-q'} * y_{d_{q'},u}^{ST,Dispatching-q'} + \sum_{\forall q' \neq q} t_{r_{q'},s,q}^{ST,Storing-q'} * y_{r_{q'},u}^{ST,Storing-q'} + \sum_{\forall p} t_{p,s,q}^{DT} * y_{p,u}^{DT} + \sum_{\forall h} f_{h,s,q} * x_{h,u} \quad \forall q,s,u \quad (4.31)$$

where  $Z_{s,q,u}$  is the composition of component u in the water assigned to sink s in time interval q.

Composition constraints for the Sinks:

$$Z_{s,q,u} \leq Z_{s,q,u}^{\max} \quad \forall q,s,u \quad (4.32)$$

where  $Z_{s,q,u}^{\max}$  is the maximum admissible composition of component u to sink s in time interval q.

Fresh flow:

$$Fresh = \sum_{\forall h} \sum_{\forall s} \sum_{\forall q} f_{h,s,q} \quad (4.33)$$

where  $f_{h,s,q}$  is the fresh water source  $h$  assigned to sink  $s$  in time interval  $q$

Pipelines:

$$w_{v,q,s}^{Direct} \leq I_{v,q,s} * J \quad (4.34)$$

$$w_{v,q,r_q}^{ST, Storing\ q} \leq I_{v,q,r_q} * J \quad (4.35)$$

$$w_{v,q,d_q'}^{ST, Dispatching\ q} \leq I_{v,q,d_q'} * J \quad (4.36)$$

$$w_{v,q,p}^{DT} \leq I_{v,q,p} * J \quad (4.37)$$

$$t_{r_q,s,q'}^{ST, Storing\ q} \leq I_{r_q,s,q'} * J \quad (4.38)$$

$$t_{d_q,s,q'}^{ST, Dispatching\ q} \leq I_{d_q,s,q'} * J \quad (4.39)$$

$$t_{p,s,q}^{DT} \leq I_{p,s,q} * J \quad (4.40)$$

where constraints 34 through 40 relate the flow to the binary integers that designate the existence of pipelines and  $J$  is the upper bound on the flow through each pipeline.

#### 4.4.4 Simplification of Network

The solution of the mathematical formulation is aimed at minimizing the total annualized cost of the network. Once the solution of the mathematical formulation and the key design and scheduling of the network have been determined, inspection of the new design is done to try to simplify the network. Some source -double tank assignments can be simplified into a source-single tank assignment. There are certain guidelines which the designer can follow in order to determine which double tank assignments can be simplified into a single tank assignment. These guidelines were not implemented as constraints in the mathematical formulation because they would be very cumbersome in a formulation view point and would require too many integers. In general, all source-double tank assignments may be simplified into a single tank assignment; however, there are some exceptions where this may not apply. The following scenarios are presented to aid the designer in determining which source-double tank assignments can not be simplified into a single tank assignment:

**1. Source supply and sink demand overlap in time interval  $q$ :** In this scenario, a set of sources supply water at different time intervals  $q$  and are allocated to a double tank assignment. The water coming from the double tanks which was supplied by the sources is allocated to a set of sinks which demand water at different time intervals  $q'$ . If storage and dispatch from this assignment is occurring over a common time interval where  $q = q'$ , then a double tank assignment is needed. Fig. 4.7 is an illustration of this scenario. If one tank were to be used in this case, then the storage and dispatch of water

in the same time interval will alter the composition of water in the tank causing it to differ from the optimal composition fed to the sink throughout period  $q'$ . Therefore, a double tank assignment is needed when storage and dispatch overlap in the same time interval unless the following is present:

- a. If all sources supplying water to the double tank arrangement are of equal composition. In this case, even though storage and dispatch is occurring over a common interval, the composition of the water in the tank will remain constant. Therefore, the double tank arrangement can be reduced to a single tank assignment.

**2. If not all sinks can be arranged between two intervals where storage is not occurring, then two tanks are needed:** In this scenario, a set of sources supply water at different time intervals  $q$  and are allocated to a double tank assignment. The water from the double tanks is supplied to sinks which demand water at different time intervals  $q'$ . If the all the  $q'$ 's can not be arranged between two  $q$  intervals  $q_i$  and  $q_{i+1}$  where storage is not occurring then two tanks are needed. Fig. 4.8 is an illustration of this scenario.

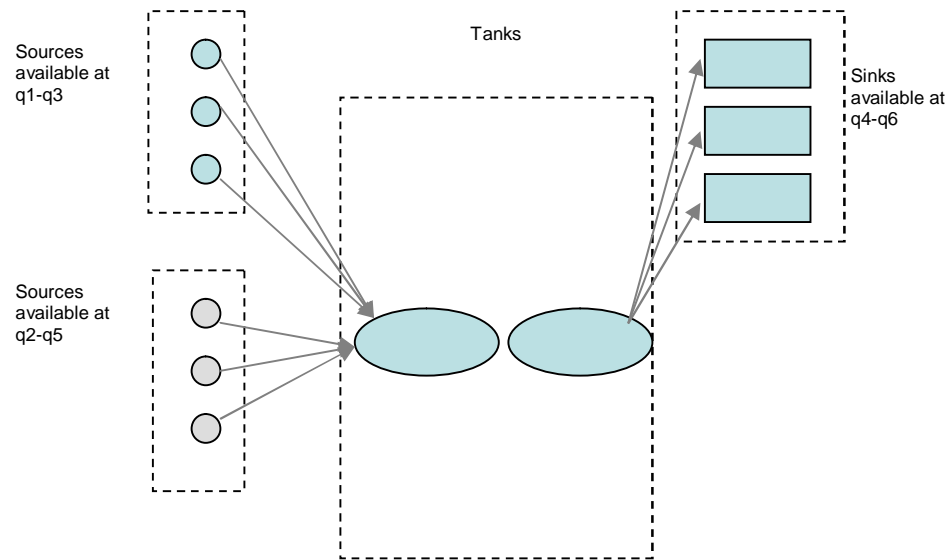


Fig. 4.7. Storage and Dispatch Occurring in the Same Time Interval

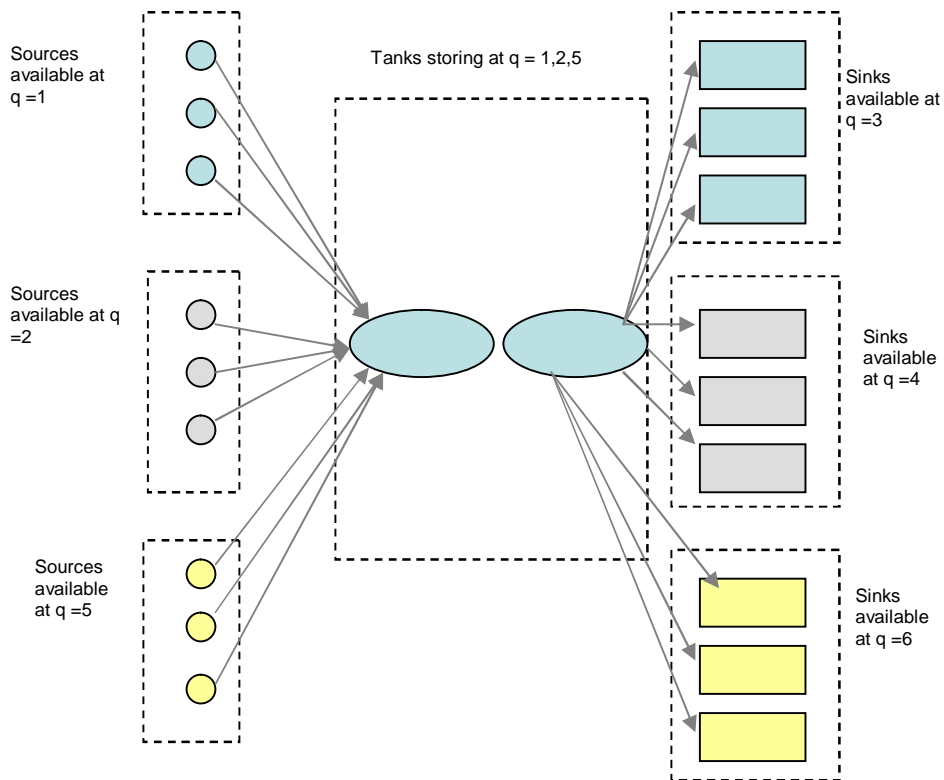


Fig. 4.8. Two Tanks are Needed When Not All Sinks Can Be Arranged  
Between Two Intervals Where Storage IS Not Occurring

#### 4.4.5 Integer Cut Constraints on Tanks

The mathematical formulation is developed to minimize the total annualized cost (TAC) of the water recycle network. Once it is solved, the designer can determine sufficient information on the design and scheduling of the cost effective network. In most cases, the network that is established from the formulation is the optimal network or is a

network which is very near the optimum. For that reason, the designer may chose to build a network established from the formulation solution. If interested, the designer may further analyze other networks to determine whether a network more superior than the formulation established network exists. This is done by implementing integer cut constraints on the tanks and resolving the formulation with the new tank constraints. Testing the extreme points first, the maximum number of tanks (predetermined by the designer) and the minimum number of tanks (zero) will be beneficial to the designer in determining whether the first solution established by the formulation is near the optimum, and which direction to begin implementing the integer cuts. The proposed approach is shown by Fig. 4.9.

First, the problem of minimizing the TAC of the network is solved using the mathematical formulation. The solution of this program provides sufficient information on the design and scheduling of the network. Next, implementing the guidelines presented in the previous section, further simplification of the network is done. The network design is inspected to see if source-double tank assignments can be scheduled in one tank. Now that the network configuration has been determined, the TAC corresponding to this system can be calculated. Next, integer cut constraints for tanks are implemented to alter the number of tanks in the network by one. The minimum TAC of the network subject to the new tank constraint is determined. Further inspection of the new design is done to try to further simplify the network. Integer cuts are continued until



they are exhausted. Solutions of the network configurations and schedules should be analyzed and the optimal solution determined.

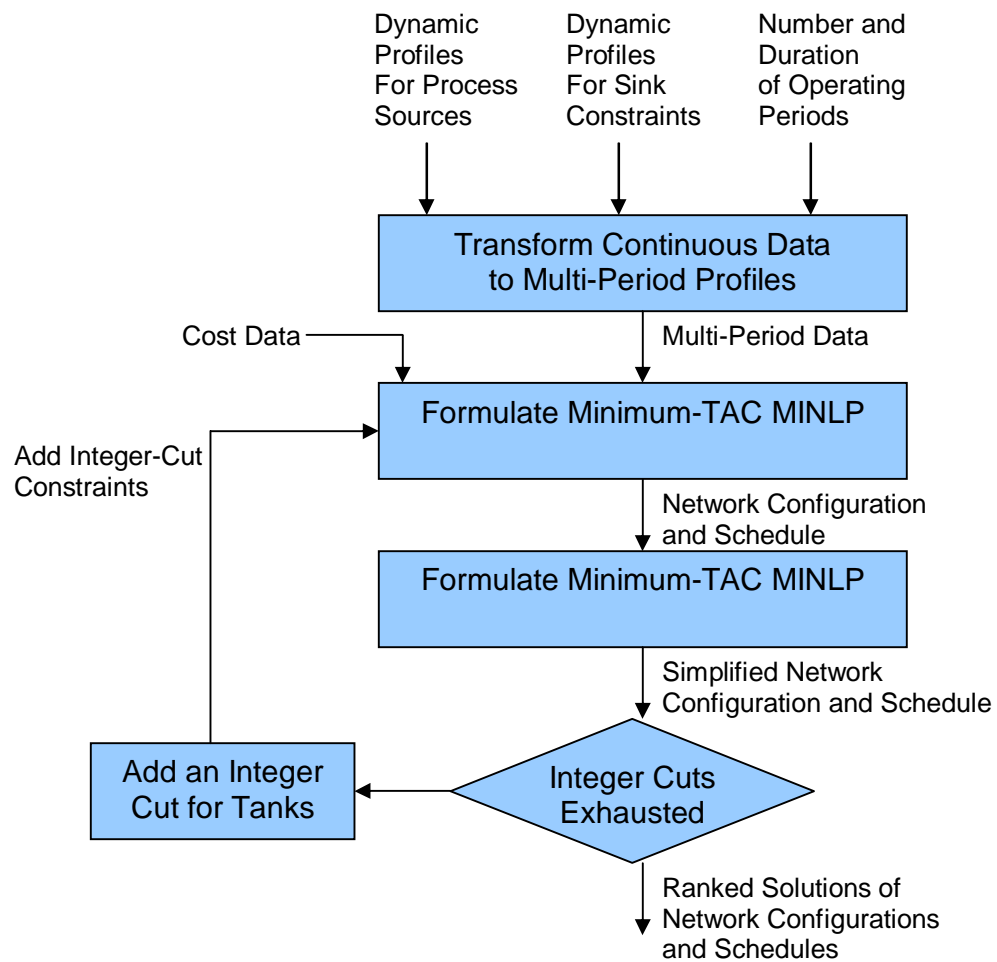


Fig. 4.9. Implementing Integer Cuts on Tanks

## 4.5 Case Study

A case study is solved to illustrate the usefulness of the devised procedure. A specialty chemical process operates in a batch mode with an eight-hour cycle time. The process is a single contaminant system that produces three recyclable water sources and has two sinks that require water usage. Because of the batch nature of the process the sources are produced over certain time periods of the cycle and the sinks require feed over specific time intervals. Tables 4.1 and 4.2 summarize the data for the sources and sinks. Available for use is one fresh water stream with a cost of \$0.20/ton of water. Also, the cost of waste water treatment is \$0.30/ton. Available are storage and dispatch tanks with an annual cost of \$35,000 per tank. Also, piping to deliver the source water to tanks, sinks, and waste storage has a cost of  $\$20/(m * year)$ . It is desired to synthesize a cost-effective water-recycle network for the following scenarios:

- a. The network operating cost is dominated by fresh water consumption and waste water generation and the fixed cost is dominated by storage and dispatch tanks.
- b. The network operating cost is dominated by fresh water consumption and waste water generation and the fixed cost is dominated by storage and dispatch tanks and piping cost.

Table 4.1

Data for the Process Sources of the Case Study (t: time (hr) from the start of the cycle)

Source Number	Function for flow rate (ton/hr)	Function for composition (ppm)	Start time (hr)	End time (hr)
1	200.00	$40 * t + 40$	0	5
2	133.33	$10 * (t - 1)^2 + 20$	1	4
3	$(15.00 * (t - 7) + 70.00) * 10$	300	7	8

Table 4.2

Data for the Process Sinks of the Case Study

Sink Number	Flow rate demand (ton/hr)	Constraint on lower bound on composition entering the sink (ppm)	Constraint on upper bound on composition entering the sink (ppm)	Start time (hr)	End time (hr)
1	290.00	0	80	1	6
2	100.00	0	350	3	7

The discretized source and sink data for this network is represented by tables 4.3, 4.4, 4.5, 4.6, and 4.7

Table 4.3

Data for the Discretized Process Sources of the Case Study

Source	Time Interval (hr)	Composition (ppm)	Flow rate (ton/hr)
1	0-1	60	200
	1-2	100	200
	2-3	140	200
	3-4	180	200
	4-5	220	200
	5-6	0	0
	6-7	0	0
	7-8	0	0
2	0-1	0	0
	1-2	70/3	133.33
	2-3	130/3	133.33
	3-4	250/3	133.33
	4-5	0	0
	5-6	0	0
	6-7	0	0
	7-8	0	0
3	7-8	300	775

Table 4.4

Data for the Discretized Process Sinks of the Case Study

Sink	Time Interval (hr)	Upper bound composition constraint (ppm)	Flow rate demand (ton/hr)
1	0-1	0	0
	1-2	80	290
	2-3	80	290
	3-4	80	290
	4-5	80	290
	5-6	80	290
	6-7	0	0
	7-8	0	0
2	0-1	0	0
	1-2	0	0
	2-3	0	0
	3-4	350	100
	4-5	350	100
	5-6	350	100
	6-7	350	100
	7-8	0	0

Table 4.5

Distance between Sources - Tanks, Sinks, and Waste of Batch Water Network

Source	Distance to Tank Facility (m)	Distance to Sink 1 (m)	Distance to Sink 2 (m)	Distance to Waste (m)
1	10	15	15	15
2	10	15	15	15
3	10	15	15	15

Table 4.6

Distance between Tank Facility and Sinks of Batch Water Network

Tank Facility	Distance to Sink 1 (m)	Distance to Sink 2 (m)
1	5	5

Table 4.7

Distance between Fresh Source and Sinks of Batch Water Network

Fresh Source	Distance to Sink 1 (m)	Distance to Sink 2 (m)
1	5	5

#### 4.5.1 Scenario I

To determine the network of minimum total annualized cost for the case where fixed cost is dominated by storage and dispatch tanks the mathematical formulation is solved. The formulation is a Mixed Integer Non-Linear Program (MINLP) consisting of 139 constraints and 418 total variables in which 197 of the total variables are nonlinear. A solution of 306.3 tons of fresh water and 631.2 tons of waste water per batch cycle with a TAC of 344,437 was found. This network is composed of two single tanks, one tank

storing at a single time interval (hour 7-8) and one tank dispatching at a single time interval (hour 5-6). Fig. 4.10 is an illustration for the proposed network.

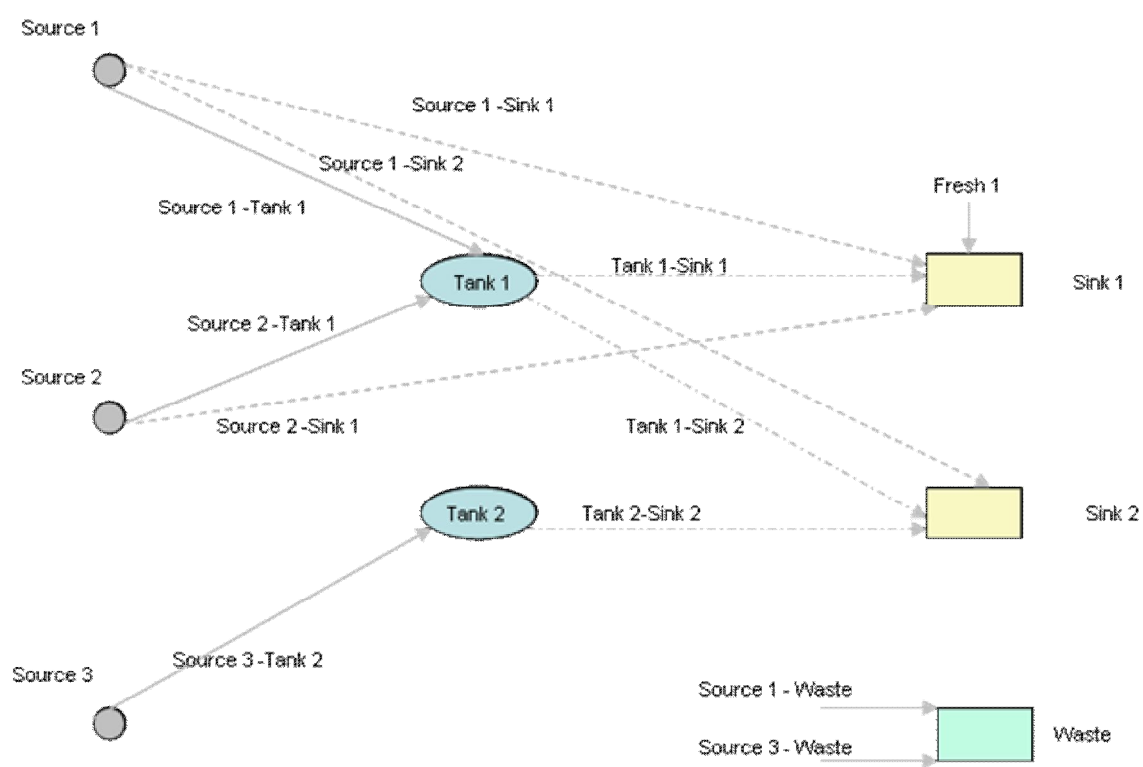


Fig. 4.10. Water Recycle Network for Scenario I

Table 4.8

Water Assignment and Scheduling Data for Fig. 4.10

Time Interval (hr)	0-1	1-2	2-3	3-4	4-5	5-6	6-7	7-8
Source1 Tank1 (Ton)	200	25.05	75.5	-----	-----	-----	-----	-----
Source1 Sink1 (Ton)	-----	175	124.45	67.2	105.45	-----	-----	-----
Source1 Sink 2 (Ton)	-----	-----	-----	100	94.54	-----	-----	-----
Source1 Waste (Ton)	-----	-----	-----	32.82	-----	-----	-----	-----
Source2 Tank1 (Ton)	-----	18.24	-----	-----	-----	-----	-----	-----
Source2 Sink1 (Ton)	-----	115.01	133.33	133.33	-----	-----	-----	-----
Source3 Tank2 (Ton)	-----	-----	-----	-----	-----	-----	-----	176.61
Source3 Waste (Ton)	-----	-----	-----	-----	-----	-----	-----	598.39
Tank1 Sink1 (Ton)	-----	-----	-----	-----	-----	290	-----	-----
Tank1 Sink2 (Ton)	-----	-----	-----	-----	-----	28.84	-----	-----
Tank2 Sink2 (Ton)	-----	-----	-----	-----	5.4545	71.15	100	-----
Fresh 1 (Ton)	-----	-----	32.25	89.52	184.54	-----	-----	-----



### 4.5.2 Scenario II

For the case where fixed cost is dominated by tank and piping cost, a MINLP formulation of 458 constraints, and 743 variables in which 694 are nonlinear and 341 are integers was solved. A solution of 306.3 tons of fresh water and 631.2 tons of waste water per batch cycle with a TAC of 346,937 was found. This network is composed of two single tanks, one tank storing at a single time interval (hour 7-8) and one tank dispatching at a single time interval (hour 5-6). Fig. 4.10 is an illustration for the proposed network.

## 4.6 Summary

This work has developed a novel systematic procedure to synthesize and schedule a cost effective batch water network. First, a structural representation has been developed to embed potential configurations. In addition to sources and sinks, two sets of tanks have been introduced for storage and dispatch. This new arrangement overcomes previous-research limitations that restricted assignment within the same batch cycle and were not capable of insuring sink feasibility when supply and demand overlap. Sources and sinks have been reformulated through discretization into meaningful events to transform simultaneous differential and algebraic equations into algebraic equations. Then, a formulation to synthesize and schedule a cost effective batch network has been developed

## **CHAPTER V**

### **A PROCESS INTEGRATION APPROACH TO THE OPTIMAL SCHEDULING OF UNSTEADY STATE MATERIAL RECOVERY NETWORKS**

#### **5.1 Introduction**

Industry at large and the chemical industry in particular are striving to improve productivity and enhance revenues in a highly competitive global economy. While much attention has been given to improving design, efficiency, and performance for individual units in chemical plants, less attention has been given to the overall integrated optimization of the processes and the overall management of resources and wastes within chemical plants. In this context, the concept of process integration can enable process engineers to develop systematic methodologies to identify integrated strategies for the optimal management and allocation of resources.

Process integration is a holistic approach to the design, operation, and scheduling of processes that emphasizes the unity of the process (El-Halwagi, 2006). This helps to maximize profitability by enhancing productivity and minimizing waste. Moreover, it contributes greatly to minimizing the negative impact of waste streams generated from chemical processes on the environment. In the area of material recovery, mass integration is a particularly effective approach that can be utilized to obtain optimal

material recovery and scheduling, enhance yield, conserve resources, debottleneck processes, mitigate environmental impact, and conserve energy. A mass-integration-based network synthesis provides cost-effective and engineering-capable solutions by addressing a set of important questions related to defining material streams and their optimal loads that need to be recycled, optimal allocation of streams that need to be routed to the process, and what kind of scheduling and arrangements need to be configured (Dunn and El-Halwagi, 2003).

Example of research in recovering materials via separation systems is the synthesis for mass exchange networks introduced by El-Halwagi and Manousiouthakis, 1989. Several categories of the problem and solution techniques have been researched (e.g., El-Halwagi and Manousiouthakis, 1990; Papalexandri, et al., 1994; Friedler et al., 1994; Garrard and Fraga, 1998; Dunn and El-Halwagi, 2003). Also, the problem of designing material recovery networks via steady-state recycle/reuse has been addressed (e.g., Wang and Smith, 1994; Keckler and Allen, 1998; Sorin and Bedard, 1999; Polley and Polley, 2000; Hallale, 2002; Savelski and Bagajewicz, 2000 a and b; Alva-Argaez', et al., 2000; Parthasarathy and Krishnagopalan, 2001; Savelski and Bagajewicz, 2001; Dunn and Wenzel, 2001; El-Halwagi et al, 2003; Foo et al., 2005).

The previous efforts focused on steady-state operations. Several important contributions have also been made in the area of batch recycle/reuse networks with special emphasis on water systems. The following are samples of these contributions. Wang and Smith,

1995, developed a time-pinch analysis method which utilizes graphical techniques to synthesize batch water networks. This work was further extended by Majozi et al., 2006. Mathematical techniques to design batch water networks were developed by Kim and Smith, 2004 and Majozi, 2005a, b. These techniques are composed of formulations which are limited to mass transfer based water units and single contaminant systems. Rabie and El-Halwagi, 2008, developed a hierarchical approach to the synthesis and scheduling of water networks.

Although previous research efforts have provided useful techniques to design material recovery networks, they have not addressed the problem of optimizing simultaneous allocation and separation of process sources for unsteady-state operations. This is a key factor in limiting the scope to recycle/reuse only without considering the role of intermediate separation systems (or interceptors).

In this work, a systematic procedure and methodology is developed to determine the optimal scheduling strategies for allocation and separation of process sources to provide value-added products. The unsteady state material recovery network involves tanks, pipelines, and interception units. The objective is to determine the optimal storage, segregation, mixing, separation, and allocation of process sources so as to maximize the process profitability while meeting all process constraints.

## 5.2 Nomenclature

Before proceeding to the problem statement and approach, it is useful to introduce the various symbols used throughout this work:

### *Indices*

$i$	process sources
$j$	products
$k$	tanks used to store sources before interception
$m$	tanks used to store sources after interception
$n$	interceptor
$q$	discretization index
$\tau$	decision making time horizon
$t$	time during period $\tau$

### *Sets*

INTERCEPTORS	units can intercept the sources in order to recover the material of interest
PRODUCTS	products with certain specifications that need to be produced from the recovered material
SOURCES	process streams containing the material of interest that needs to be recovered
TANKS 1	tanks used to store the sources before interception
TANKS 2	tanks used to store sources after interception

### Parameters

$Cost_{interceptor}$	operating cost of interceptor
$Cost_{waste}$	cost of waste treatment
$Nt$	number of discretization time intervals spanning time period $\tau$
$Price_{product}$	selling price for produced product
$\lambda_{ethanol}$	latent heat of ethanol
$\lambda_{water}$	latent heat of water

### Variables

$A_{i,q}$	the quantity of discretized source $i$ in time interval $q$
$a_{i,k,q}$	the amount of source $i$ dispatched to tank $k$ during time period $q$
$a_{i,waste,q}$	the amount of source $i$ dispatched to waste during time period $q$
$b_{k,n,q}$	is the flow rate entering interception $n$ from tank $k$ at time interval $q$
$c_{n,o,j,q}$	quantity of stream $o$ exiting interception unit $n$ during time period $q$ that will be dispatched to product inventory $j$
$c_{n,o,m,q}$	quantity of stream $o$ exiting interception unit $n$ during time period $q$ that will be stored in tank $m$
$c_{n,o,n',q}$	is the flow rate exiting interception $n$ dispatched to interception $n'$ where $n \neq n'$ at time $q$
$c_{n,o,waste,q}$	is the flow rate exiting interception $n$ dispatched to waste
$d_{m,j,q}$	flow leaving tank $m$ during time period $q$ to product inventory $j$
$d_{m,n,q}$	flow leaving tank $m$ during time period $q$ to interception unit $n$

$F_{n,q}^{in}$	flow rate entering interception unit $n$ during time period $q$
$F_{n,o,q}^{out}$	flow rate exiting interceptor unit $n$ during time period $q$ from intercepted stream $o$
$h_B$	enthalpy of the bottoms stream of the stripper
$h_D$	enthalpy of the distillate stream of the stripper
$h_F$	enthalpy of the feed stream of the stripper
$P_{j,q}$	quantity of product inventory $j$ over interval $q$
$P_{j,q}^{\max}$	maximum quantity constraint on product inventory $j$ over interval $q$
$P_{j,q}^{\min}$	minimum quantity constraint on product inventory $j$ over interval $q$
$Q_{condenser}$	heating duty of the condenser
$Q_{Heater}$	heating duty of the heater
$Q_{Reboiler}$	heating duty of the reboiler
$T_{k,q}^1$	the total quantity of the material stored in tank $k$ during time period $q$
$T_{k,q-1}^1$	the total inventory remaining in tank $k$ from time period $q-1$
$T_{m,q}^2$	is the total quantity of the material stored in tank $m$ during time period $q$
$T_{m,q-1}^2$	the total inventory remaining in tank $m$ from time period $q-1$
$V_{i,q}$	the composition of the material of interest from sources $i$ during time period $q$
$Waste$	total material dispatched to waste

$W_{k,q}$	the composition of the material of interest in tank $k$ during time period $q$
$W_{k,q-1}$	the composition of the material of interest in tank $k$ during time period $q-1$
$X_{ethanol}$	ethanol composition in stream entering heater
$X_{n,q}^{in}$	composition of the desired material in the stream entering interception unit $n$ at time period $q$
$X_{n,o,q}^{out}$	composition of the desired material exiting interception unit $n$ from intercepted stream $o$ at time period $q$
$Y_{m,q}$	is the composition of the material of interest in tank $m$ during time period $q$
$Y_{m,q-1}$	is the composition of the material of interest in tank $m$ during time period $q-1$
$Z_{j,q}$	composition of product inventory $j$ over interval $q$
$Z_{j,q}^{\max}$	the maximum composition constraint on product inventory $j$ over interval $q$
$Z_{j,q}^{\min}$	the minimum composition constraint on product inventory $j$ over interval $q$



### 5.3 Problem Statement

The material recovery network problem to be addressed in this work may be stated as follows:

Given is a process with a number of interception units, tanks, and pipelines. The process receives various batches of feedstocks that are to be processed to produce a number of value-added/higher quality products that meet certain market demands. It is desired to determine optimal scheduling strategies for the allocation and separation of the feedstocks over a decision making time horizon  $\tau$ . The above is characterized by the following:

- Sources: There is a set of sources  $SOURCES = \{i|i = 1, 2, \dots, N_{SR}\}$  of process streams containing the material of interest that needs to be recovered. The dynamic profiles for the flow rate and composition of each source,  $i$ , are known only over  $\tau$  and given by  $a_i(t)$  and  $v_i(t)$  where  $t$  is the time during period  $\tau$ .
- Interceptors: There is a set of existing interceptor units  $INTERCEPTORS = \{n|n = 1, 2, \dots, N_{INT}\}$  with a set type, size, and design. These units can intercept the sources in order to recover the material of interest. There are also capacity and composition limitations on the feed to each interceptor and are given by

$$F_n^{in, \min} \leq F_n^{in} \leq F_n^{in, \max} \text{ and } X_n^{in, \min} \leq X_n^{in} \leq X_n^{in, \max} \text{ respectively.}$$

- Tanks: There are two sets of tanks  $TANKS\ 1 = \{ k | k = 1, 2, \dots, N_{TK1} \}$  and  $TANKS\ 2 = \{ m | m = 1, 2, \dots, N_{TK2} \}$  with a set location and capacity. TANKS 1 can be used to store the sources before interception and have a capacity  $T_k^1$ . TANKS 2 store sources after interception and have a capacity  $T_m^2$ .
- Products: There is a set of products  $PRODUCTS = \{ j | j = 1, 2, \dots, N_{PD} \}$  with certain specifications that need to be produced from the recovered material. The flow rate and composition constraints on the desired product are given by:

$$P_j^{\min}(t) \leq P_j(t) \leq P_j^{\max}(t) \text{ and } Z_j^{\min}(t) \leq Z_j(t) \leq Z_j^{\max}(t)$$

The objective is to develop a systematic procedure to determine the optimal scheduling schemes for the optimal material recovery network over time period  $\tau$  in which sources may be stored in tanks, mixed, and/or intercepted to produce the desired products. The material recovery network must produce the maximum profits and meet all process constraints.

## 5.4 Approach

The following procedure is proposed:

1. Multi-period reformulation of the process over time period  $\tau$ .

2. Development of a structural representation to embed network configurations of interest for scheduling.
3. Derivation of optimal performance policies of the interception units.
4. Development of mathematical formulations which include interceptor performance equations for each discrete time interval within time period  $\tau$ .
5. All mathematical formulations over time period  $\tau$  are solved simultaneously utilizing parametric optimization aimed at maximizing total annualized profit of the network while determining key scheduling information.

#### 5.4.1 Multi-Period Reformulation of the Process

Due to the dynamic variation of the sources, the problem will be transformed into a multi-period problem with discrete time intervals  $q$  spanning time period  $\tau$ . The sources, interceptors, and tanks will all be discretized into a number  $N_t$  of time intervals spanning time period  $\tau$ . The time intervals will be small enough to capture significant changes in flow rate and composition, but large enough to keep the problem from becoming too cumbersome. The discretization index is referred to as  $q$  where the  $q^{th}$  time interval between indices  $q-1$  and  $q$  is described by the following time interval  $[t_{q-1} \text{ and } t_q]$ . The flow rate profile of each source,  $i$ , is transformed into a discrete set of flows (water quantities per cycle not continuous flow rates). For the  $q^{th}$  time interval, the quantity of the  $i^{th}$  source is given by:

$$A_{i,q} = \int_{t_{q-1}}^{t_q} a_i(t) dt \quad (5.1)$$

and the composition of the material of interest in source  $i$  in time interval  $q$  is given by:

$$V_{i,q} = \frac{\int_{t_{q-1}}^{t_q} a_i(t) v_i(t) dt}{A_{i,q}} \quad (5.2)$$

A similar discretization is performed for the flow rate and constraints of the product specifications. For the interceptor units, the time domain is also decomposed into a number  $N_t$  of time intervals spanning the cycle time  $\tau$ . For each discrete time interval  $q$ , the performance equations for the flow entering and exiting the interceptor unit are given by:

$$F_{n,q}^{in} = f(b_{k,n,q}, c_{n',n,q}, d_{m,n,q}) \quad (5.3)$$

where  $F_{n,q}^{in}$  is the total flow rate entering interception  $n$  at time interval  $q$ ,  $b_{k,n,q}$  is the flow rate entering interception  $n$  from tank  $k$  at time interval  $q$ ,  $c_{n',n,q}$  is the flow rate entering interception  $n$  from interception  $n'$  where  $n \neq n'$  at time  $q$ , and  $d_{m,n,q}$  is the flow rate entering interception  $n$  from tank  $m$  at time interval  $q$ .

$$F_{n,o,q}^{out} = f(F_{n,q}^{in}, W_{k,n,q}, X_{n',n,q}, Y_{m,n,q}, \text{OperationalConditions}) \quad (5.4)$$

where  $F_{n,o,q}^{out}$  is the flow rate exiting interception unit  $n$  at time interval  $q$ ,  $F_{n,q}^{in}$  is the total flow rate entering the interception unit  $n$  at time interval  $q$ ,  $W_{k,n,q}$  is the composition of the material entering interception unit  $n$  from tank  $k$  at time interval  $q$ ,  $X_{n',n,q}$  is the composition of the material entering interception unit  $n$  from interception  $n'$  at time interval  $q$ , and  $Y_{m,n,q}$  is the composition of the material entering interception unit  $n$  from tank  $m$  at time interval  $q$ .

The composition of the desired material in the stream entering and exiting interception unit  $n$  is given by:

$$X_{n,q}^{in} = f(W_{k,n,q}, X_{n',n,q}, Y_{m,n,q}, F_{n,q}^{in}) \quad (5.5)$$

$$X_{n,o,q}^{out} = f(X_{n,q}^{in}, F_{n,q}^{in}, \text{OperationalConditions}) \quad (5.6)$$

where  $W_{k,n,q}$  is the composition of the flow coming from tank  $k$ ,  $X_{n',n,q}$  is the composition of the flow coming from interception unit  $n'$  where  $n' \neq n$ ,  $Y_{m,n,q}$  is the composition coming from tank  $m$ , and  $F_{n,q}^{in}$  is the total flow entering interception unit  $n$ . The outlet composition exiting interception  $n$  is a function of the total inlet

composition  $X_{n,q}^{in}$  to interception  $n$ , the total flow rate  $F_{n,q}^{in}$  entering interception  $n$ , and the operational conditions of the interceptor.

#### 5.4.2 Structural Representation

The next step to schedule an optimal material recovery network is developing a structural representation which embeds all potential configurations of the network and enables proper scheduling. As illustrated by Fig. 5.1, source  $i$  over time period  $q$  may be stored in tanks  $k$ , intercepted, sent to waste, or sent to product inventory. Streams exiting interception unit  $n$  may be sent directly to interception unit  $n'$  where  $n' \neq n$ , stored in tanks  $m$ , or sent directly to product inventory. Stored ethanol in tanks  $m$  may be sent back for further interception or sent to product inventory.

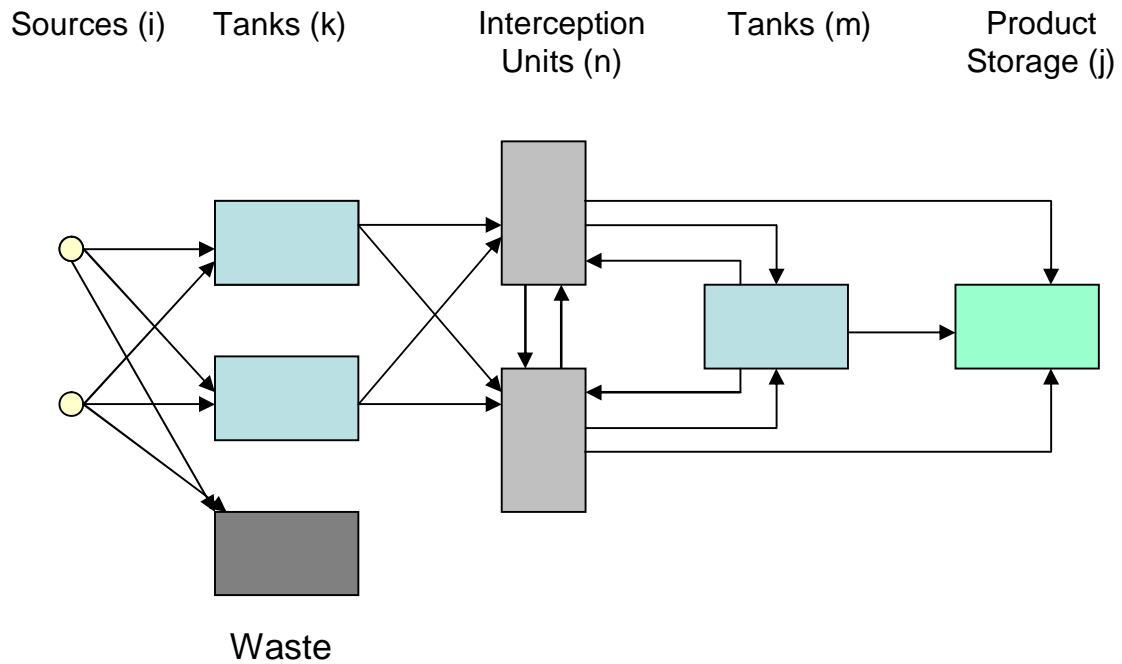


Fig. 5.1. Source-Tank-Interceptor-Tank Representation

#### 5.4.3 Derivation of Optimal Policies for the Interception Units

A primary challenge in the optimization formulation and solution of the scheduling problem at hand is the need to optimize the operation of the interception (e.g., separation) in the midst of the overall optimization formulation. Specifically, there are two key challenges:

- a. The performance of the units may not be available in the form of explicit mathematical model that can be incorporated in a deterministic optimization

formulation. A common example is when the units are modeled via a computer-aided simulation package.

b. The optimization of operating conditions (such as reflux ratio and reboiler duty for a distillation column) can be difficult when the feed flow rate and composition are unknown and are still to be determined by the context of the overall scheduling.

To overcome both challenges, we invoke Bellman's principle of optimality (dynamic programming) which states that "an optimal policy has the property that, whatever the initial state and the initial decision are, the remaining decisions must constitute an optimal policy with regard to the state resulting from the first decision." (Bellman, 1957). Consequently, propose the following two-stage approach:

1. Derivation of optimal operating policies for the interception units: This step is carried out before the overall optimization of the material recovery network. Even if the performance of the interception devices is not available as an explicit mathematical model but is modeled via a computer-aided simulation, the model is run for various feed flow rates and compositions. For each combination of feed flow rate and composition, the optimal set of operating variables is determined. The exercise is repeated for various pairs of feed flow rate and composition and the optimal variables are identified for each pair. Then, regression analysis is carried out to derive a parametric optimal policy for the operating variables of each interception unit as a function of feed flow rate and composition.



2. The derived optimal policies are included in the overall optimization problem for allocation and separation. Because the optimal policies are derived parametrically and without commitment to specific feed conditions, their inclusion in the overall formulation is consistent with Bellman's optimality principle.

#### 5.4.4 Mathematical Formulations

The next step is to formulate an optimization program whose solution will provide sufficient information to schedule an optimal material recovery network. As mentioned above, the process is decomposed into a number of time intervals  $N_t$  with discrete time intervals  $q$  spanning time period  $\tau$ . For each time interval  $q$ , a set of equations will be developed relating the sources, tanks, interception units, and desired products. The equations for every  $q$  will be related to one objective function and simultaneously solved to obtain the optimal scheduling scenario. The objective function is the following:

$$\text{Maximize Profit} = \text{Price}_{\text{product}} * \sum_q P_{j,q} - \text{Cost}_{\text{interception}} f(\text{OperationalConditions}) - \text{Cost}_{\text{waste}} * \text{Waste} \quad (5.7)$$

where  $\text{Price}_{\text{product}}$ ,  $\text{Cost}_{\text{interception}}$ , and  $\text{Cost}_{\text{waste}}$  are the selling price coefficient for the recovered material, cost coefficient for intercepting source streams containing the material of interest, and the cost coefficient for the waste treatment respectively. Also

$\sum_q P_{j,q}$  is the total material recovered and  $Waste$  is the total waste produced over time period  $\tau$ .

Source Balances:

$$A_{i,q} = \sum_k a_{i,k,q} + a_{i,waste,q} \quad \forall i, q \quad (5.8)$$

where  $A_{i,q}$  is the quantity of discretized source  $i$  in time interval  $q$ ,  $a_{i,k,q}$  is the amount of source  $i$  dispatched to tank  $k$  during time period  $q$ , and  $a_{i,waste,q}$  is the amount of source  $i$  dispatched to waste during time period  $q$ .

Tank Balances for storing sources:

$$T_{k,q}^1 = T_{k,q-1}^1 + \sum_i a_{i,k,q} - \sum_n b_{k,n,q} \quad \forall k, q \quad (5.9)$$

where  $T_{k,q}^1$  is the total quantity of the material stored in tank  $k$  during time period  $q$  and it is equal to  $T_{k,q-1}^1$  the total inventory remaining in tank  $k$  from time period  $q-1$ ,  $a_{i,k,q}$  the sum of all the sources dispatched to tank  $k$  during time period  $q$ , and  $\sum_n b_{k,n,q}$  all the stored material leaving tank  $k$  during time period  $q$ .

$$T_{k,q}^1 * W_{k,q} = T_{k,q-1}^1 * W_{k,q-1} + \sum_i a_{i,k,q} * V_{i,q} - \sum_n b_{k,n,q} * W_{k,q} \quad \forall k, q \quad (5.10)$$

where  $W_{k,q}$  is the composition of the material of interest in tank  $k$  during time period  $q$ ,  $W_{k,q-1}$  is the composition of the material of interest in tank  $k$  during time period  $q-1$ , and  $V_{i,q}$  is the composition of the material of interest coming from sources  $i$  being dispatched to tank  $k$  during time period  $q$ .

Interceptor Balances:

$$F_{n,q}^{in} = \sum_k b_{k,n,q} + \sum_{\forall o} \sum_{\forall n', n \neq n'} c_{n',o,n,q} + \sum_m d_{m,n,q} \quad \forall n, q \quad (5.11)$$

where the total flow rate entering interception unit  $n$  during time period  $q$   $F_{n,q}^{in}$ , is equal

to  $\sum_k b_{k,n,q}$  the total flow of material coming from tanks  $k$  during time period  $q$ ,

$\sum_{\forall o} \sum_{\forall n', n \neq n'} c_{n',o,n,q}$  the total flow of material coming from interception units  $n'$  where

$n' \neq n$  during time period  $q$ , and  $\sum_m d_{m,n,q}$  the total flow of material coming from tanks

$m$  during time period  $q$ .

$$F_{n,q}^{in} * X_{n,q}^{in} = \sum_k b_{k,n,q} * W_{k,q} + \sum_{\forall o} \sum_{\forall n', n \neq n'} c_{n',o,n,q} * X_{n',o,q}^{out} + \sum_m d_{m,n,q} * Y_{m,q} \quad \forall n, q \quad (5.12)$$

where  $X_{n,q}^{in}$  is the total composition of the material entering interception unit  $n$  during time period  $q$ ,  $X_{n',o,q}^{out}$  is the composition of the stream entering interception unit  $n$  coming from interception unit  $n'$  where  $n' \neq n$ , and  $Y_{m,q}$  is the composition of the stream coming from tank  $m$ .

$$F_{n,o,q}^{out} = f(F_{n,q}^{in}, X_{n,q}^{in}, \text{OperationalConditions}) \quad (5.13)$$

where  $F_{n,o,q}^{out}$  is the outlet stream  $o$  exiting interception unit  $n$  during time period  $q$  and is a function of the inlet flow rate  $F_{n,q}^{in}$ , the inlet composition  $X_{n,q}^{in}$ , and the operational conditions of the unit.

$$X_{n,o,q}^{out} = f(F_{n,q}^{in}, X_{n,q}^{in}, \text{OperationalConditions}) \quad (5.14)$$

where  $X_{n,o,q}^{out}$  is the outlet composition of stream  $o$  exiting interception unit  $n$  during time period  $q$  and is a function of the inlet flow rate  $F_{n,q}^{in}$ , the inlet composition  $X_{n,q}^{in}$ , and the operational conditions of the unit.

$$F_{n,o,q}^{out} = \sum_m c_{n,o,m,q} + \sum_{\forall n', n' \neq n} c_{n,o,n',q} + c_{n,o,waste,q} + \sum_j c_{n,o,j,q} \quad \forall n, o, q \quad (5.15)$$

where  $c_{n,o,m,q}$ ,  $c_{n,o,n',q}$ ,  $c_{n,o,waste,q}$  and  $c_{n,o,j,q}$  are the quantities of stream  $o$  exiting interception unit  $n$  during time period  $q$  that will be stored in tank  $m$ , sent to interception unit  $n'$ , sent to waste, or dispatched to product inventory  $j$ .

Tank balances for storing intercepted sources:

$$T_{m,q}^2 = T_{m,q-1}^2 + \sum_n \sum_o c_{n,o,m,q} - \sum_n d_{m,n,q} - \sum_j d_{m,j,q} \quad \forall m, q \quad (5.16)$$

where  $T_{m,q}^2$  is the total quantity of the material stored in tank  $m$  during time period  $q$  which is equal to  $T_{m,q-1}^2$  the total inventory remaining in tank  $m$  from time period  $q-1$ ,  $\sum_n \sum_o c_{n,o,m,q}$  the sum of all the intercepted source streams  $o$  from units  $n$  dispatched to tank  $m$  during time period  $q$ , minus  $\sum_n d_{m,n,q}$  the sum of all the stored material dispatched from tank  $m$  during time period  $q$  to interception units  $n$ , and  $\sum_j d_{m,j,q}$  the sum of all the material leaving tank  $m$  during time period  $q$  to product inventory  $j$ .

$$T_{m,q}^2 * Y_{m,q} = T_{m,q-1}^2 * Y_{m,q-1} + \sum_n \sum_o c_{n,o,m,q} * X_{n,o,q}^{out} - \sum_n d_{m,n,q} * Y_{m,q} - \sum_j d_{m,j,q} * Y_{m,q} \quad \forall m, q \quad (5.17)$$

where  $Y_{m,q}$  is the composition of the material of interest in tank  $m$  during time period  $q$ ,  $Y_{m,q-1}$  is the composition of the material of interest in tank  $m$  during time period  $q-1$ ,

and  $X_{n,o,q}^{out}$  is the composition of the stored source stream  $o$  from interception units  $n$  in tank  $m$  during time period  $q$ .

Waste balances:

$$Waste = \sum_i \sum_q a_{i,waste,q} + \sum_n \sum_o \sum_q c_{n,o,waste,q} \quad (5.18)$$

where the total waste is coming from  $\sum_i \sum_q a_{i,waste,q}$  and  $\sum_n \sum_o \sum_q c_{n,o,waste,q}$ , the sum of all waste coming from source streams  $i$  and the sum of all waste coming from outlet streams  $o$  of interception units  $n$  respectively.

Product balances:

$$P_{j,q} = \sum_n \sum_o c_{n,o,j,q} + \sum_m d_{m,j,q} \quad \forall j,q \quad (5.19)$$

where  $P_{j,q}$  is the total product  $j$  inventory in time interval  $q$

$$P_{j,q} * Z_{j,q} = \sum_n \sum_o c_{n,o,j,q} * X_{n,o,q}^{out} + \sum_m d_{m,j,q} * Y_{m,q} \quad \forall j,q \quad (5.20)$$

where  $Z_{j,q}$  is the composition of the total product  $j$  inventory in time interval  $q$

Product specifications on flows and compositions:

$$P_{j,q}^{\min} \leq P_{j,q} \leq P_{j,q}^{\max} \quad \forall j, q \quad (5.21)$$

$$Z_{j,q}^{\min} \leq Z_{j,q} \leq Z_{j,q}^{\max} \quad \forall j, q \quad (5.22)$$

where  $P_{j,q}^{\min}$ ,  $P_{j,q}^{\max}$ ,  $Z_{j,q}^{\min}$  and  $Z_{j,q}^{\max}$  are the minimum and maximum flow and composition constraints on product inventory  $j$  over interval  $q$ .

## 5.5 Case Study

A case study is solved to illustrate the usefulness of the devised procedure. A plant produces ethanol (material of interest) to be used as a feed to an ethanol dehydration unit (molecular sieve) that produces fuel-grade ethanol to be blended with gasoline. The process receives sugar-containing liquids (e.g., beverage waste) that are fermented to produce ethanol. The process may also receive ethanol-containing wastes. The plant contains three storage tanks, a heater and two interception units, the first being a stripping column and the second is a rectifier column (Fig.5.2).

The plant manager is in need to develop a short-term scheduling strategy over a time horizon of six days to obtain the desired ethanol recovery at minimum cost to the plant.

Over the next six days, three sources resulting from fermentation are available.

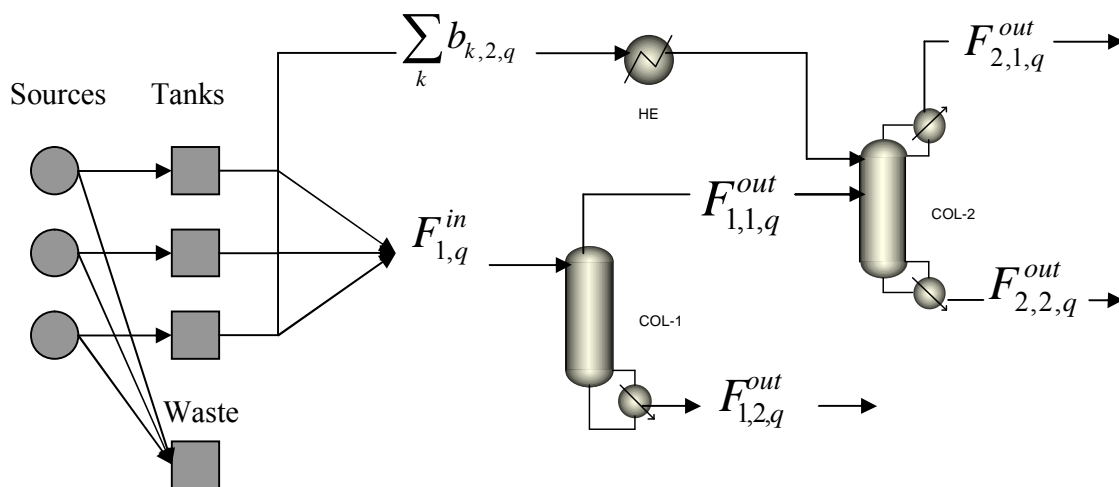


Fig. 5.2. Ethanol Recovery Process

When each source becomes available from the fermentation process, it is stored in a separate tank. Once stored, each source can be sent directly to the first interception unit (stripper), if the ethanol concentration is high enough the source may be sent to the second interception unit (rectifier), and the unused sources are sent to waste. The stream



$F_{1,1,q}^{out}$  exiting the first interception unit is a vapor stream and it is sent directly to the rectifier.

Ethanol streams entering the rectifier and coming directly from the storage tanks must be vaporized first using a heater before entering the column. Also, the inlet composition of the ethanol stream entering the first interception unit must fall within the following compositions  $6\% \leq X_{1,q}^{in} \leq 64\%$ , and the inlet composition of the stream entering the second interception unit must fall between the following compositions  $32 \leq X_{2,q}^{in} \leq 94\%$ .

Once the superstructure of the process is created, the next step in the solution is the discretization. The six-day time horizon is discretized into three time intervals  $q$ , where  $q = 1$  is the time interval designating day one and day two. Table 5.1 summarizes the desired product specifications within each discrete interval and Table 5.2 illustrates when the three sources will become available and their quantities during each time interval.

Table 5.1

Data for the Product Specifications

Day	Quantity (tons)	Minimum Grade (% ethanol)
1-2	300	92
3-4	200	92
5-6	200	92

Table 5.2

Data for the Flow of Sources Over a Six Day Time Horizon

Source	q = 1 (day 1-2)	q = 2 (day 3-4)	q = 3 (day 5-6)
Source 1 (6% ethanol)	7000 tons		
Source 2 (16% ethanol)		1500 tons	
Source 3 (8% ethanol)			2000 tons

The following are the performance equations and optimal policies for the two interception units:

Stripper performance equations:

$$X_{1,1,q}^{out} = .868 * (X_{1,q}^{in})^{.313} \quad (5.23)$$

$$F_{1,1,q}^{out} (ton / day) = (X_{1,q}^{in} / X_{1,1,q}^{out}) * Ethanol Recovery * F_{1,q}^{in} \quad (5.24)$$

$$Optimal Ethanol Recovery = 1 - (.04) * \exp(-.06 * X_{1,q}^{in}) \quad (5.25)$$

$$Q_{Re boiler} (BTU / day) = (h_B - h_F) * (F_{1,q}^{in}) + (h_D - h_B) * F_{1,1,q}^{out} \quad (5.26)$$

$$h_F (BTU / ton) = -9851.4 * X_{1,q}^{in} + 15667 \quad (5.27)$$

$$h_D (BTU / ton) = -7742.8 * X_{1,1,q}^{out} + 16667 \quad (5.28)$$

$$h_B (BTU / ton) = -9851.4 * X_{1,2,q}^{out} + 15667 \quad (5.29)$$

Rectifier performance equations:

$$X_{2,1,q}^{out} = 1 - 0.06 * \exp(0.8 * (0.71 - X_{2,q}^{in})) \quad (5.30)$$

$$F_{2,1,q}^{out} (ton / day) = (X_{2,q}^{in} / X_{2,1,q}^{out}) * Ethanol Recovery * F_{2,q}^{in} \quad (5.31)$$

$$Optimal Ethanol Recovery = (1 - 0.03) * \exp(-0.08 * X_{2,q}^{in}) \quad (5.32)$$

$$Q_{condenser} (BTU / day) = 5.641 * 10^5 + (5.65 * 10^4) * (F_{2,q}^{in}) + (-3.384 * 10^6) * X_{2,q}^{in} \quad (5.33)$$

$$Q_{Reboiler} (BTU / day) = 7.276 * 10^5 + (4.254 * 10^4) * (F_{2,q}^{in}) + (-2.038 * 10^6) * X_{2,q}^{in} \quad (5.34)$$

Heater performance equation:

$$Q_{Heater} (BTU / day) = Flow [\lambda_{ethanol} * X_{ethanol} + \lambda_{water} * (1 - X_{ethanol})] \quad (5.35)$$

$$\lambda_{ethanol} = 34,753,733 BTU / ton \quad (5.36)$$

$$\lambda_{water} = 1,944,713 BTU / ton \quad (5.37)$$

The utility cost for the reboiler on the stripper, rectifier, and heater is  $\$8/MMBTU$  and the utility cost for the condenser on the rectifier is  $\$12/MMBTU$ . It is desired to schedule an optimal ethanol recovery network with the desired ethanol production rate and grade.

An MINLP with 53 constraints, in which 23 are non linear constraints and 52 variables, was solved using the Global Solver option of the software LINGO. An optimum scheduling scheme which corresponds to a network with a minimum operating cost of \$1,669 over the six-day period was determined. Fig. 5.3 and Table 5.3 illustrate the scheduling scheme found.

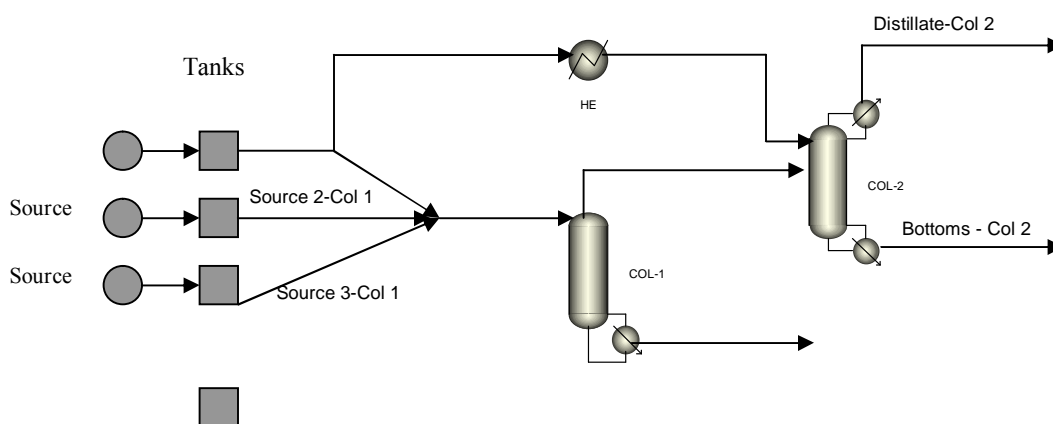


Fig. 5.3. Scheduling Scheme for Ethanol Plant

Table 5.3

## Scheduling Data for Ethanol Plant

Time Interval q	1	2	3
Source 1 to Col 1	4935 tons	355 tons	34 tons
Source 2 to Col 1	0	1100 tons	400 tons
Source 3 to Col 1	0	0	1642 tons
Ethanol Recovery Col 1	96.01%	96.00%	96.02%
Feed to Col 1	4935 tons	1455 tons	2076 tons
Distillate of Col 1	790 tons	408 tons	456 tons
Bottoms of Col 1	4145 tons	1047 tons	1620 tons
Feed to Col 2	790 tons	408 tons	456 tons
Distillate of Col 2	300 tons	199 tons	199 tons
Bottoms of Col 2	490 tons	209 tons	257 tons
Ethanol Recovery Col 2	97.09%	97.10%	97.09%
Inventory of Source 1	2065 tons	1710 tons	1676 tons
Inventory of Source 2	0	400 tons	0
Inventory of Source 3	0	0	358 tons

## 5.6 Summary

This work considered the problem of scheduling the operation of a process receiving time-varying feedstocks to yield products with desired specifications. A systematic procedure and methodology was developed to schedule and operate an unsteady state material recovery network with given tanks, pipelines, and interception units. The objective is to determine the storage, allocation, and separation of the various sources over time so as to achieve maximum profitability while meeting all process constraints. Due to the dynamic variation of the sources, the problem was transformed into a multi-period problem with discrete time intervals  $q$  spanning time period  $\tau$ . The sources, interceptors, and tanks were discretized into a number  $N_t$  of time intervals spanning the cycle time  $\tau$ .

A structural representation was developed to embed the network configurations of interest for scheduling. Bellman's principle of optimality was used as the basis for a two-stage optimization formulation. In the first stage, parametric optimization is carried out to determine the optimal policies for operating each interception device. Next, these optimal policies are incorporated in an optimization formulation that seeks to optimally schedule the storage, mixing, and interception of sources. The mathematical formulations over time period  $\tau$  were solved simultaneously for the discretized periods to achieve total annualized profit of the network while determining key scheduling

information. A case study involving the recovery of ethanol was solved to illustrate the usefulness of the devised procedure.



## **CHAPTER VI**

### **CONCLUSIONS**

The research presented in this dissertation develops systematic methodologies and novel approaches to achieve a fundamental understanding and provide cost-effective solutions for problems related to unsteady state material recovery networks. Particularly, it focuses on the following two areas: synthesis and scheduling of optimal batch water-recycle networks, and optimal scheduling of unsteady state material recovery networks with interception units.

In regards to batch water recycle networks, two novel systematic procedures to synthesize and schedule cost-effective batch water networks were developed. Both procedures introduce a new double tank arrangement that allows for storage and dispatch in subsequent cycles. This new arrangement overcomes previous-research limitations that restricted assignment within the same batch cycle and were not capable of insuring sink feasibility when supply and demand overlap. The first developed methodology is a hierarchical procedure involving multiple steps. The first step determines minimum targets for both fresh water consumption and waste water discharge ahead of network design. Utilizing benchmarks determined in the first step, a MINLP is solved to determine the minimum fixed cost network subject to the minimum targets determined in the first step. Finally, an iterative procedure has been established to trade off operating

and fixed costs (e.g., by iteratively trading off fresh water consumption and number of tanks) until the network of minimum TAC is identified.

The second methodology developed for the synthesis and scheduling of cost-effective batch water networks is a one step simultaneous approach. First, a structural representation has been developed to embed potential configurations. These configurations include direct recycle of sources to sinks, recycle of sources to sinks utilizing a single tank, and recycle of sources to sinks utilizing a double tank arrangement allowing for storage and dispatch in subsequent cycles. Then, a formulation was developed to synthesize and schedule a cost-effective batch network which includes all the potential configurations of water recycle and has an objective function that minimizes both the operating and fixed cost of the network. Once the formulation is solved information on the design and scheduling of the cost-effective network becomes available.

The second focus of this research is the development of a systematic procedure for the optimal scheduling of unsteady state material recovery networks with interception units. The network of interest has an existing design and location for tanks, pipelines, and interception units. First, the problem was transformed into a multi-period problem with discrete time intervals  $q$  spanning time period  $\tau$ . The sources, interceptors, and tanks were discretized into a number  $N_t$  of time intervals spanning the cycle time  $\tau$ .

Then a structural representation was developed to embed the network configurations of interest for scheduling, and explicit modeling of interceptor units was done through simulation, observation, and regression to develop performance equations for each interceptor unit. Moreover, mathematical formulations were developed to optimally schedule the storage, mixing, and interception of sources. The mathematical formulations over time period  $\tau$  were solved simultaneously utilizing parametric optimization aimed at maximizing total annualized profit of the network while determining key scheduling information. A case study involving the recovery of ethanol was solved to illustrate the usefulness of the devised procedure.

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